



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 10:25 PM GMT

PDB ID : 1TL1  
Title : CRYSTAL STRUCTURE OF HIV-1 REVERSE TRANSCRIPTASE IN  
COMPLEX WITH GW451211  
Authors : Hopkins, A.L.; Ren, J.; Stuart, D.I.; Stammers, D.K.  
Deposited on : 2004-06-09  
Resolution : 2.90 Å(reported)

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

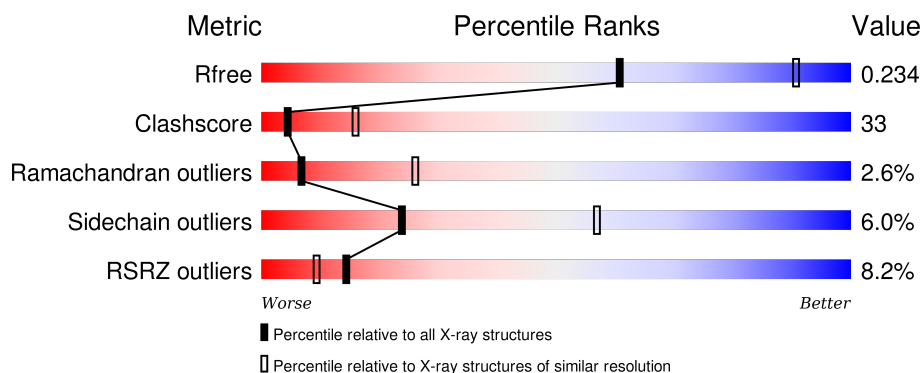
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.90 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	1451 (2.90-2.90)
Clashscore	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)
RSRZ outliers	91569	1456 (2.90-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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
4	H18	A	999	-	-	-	X

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 7604 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 CYS	UNP P04585

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

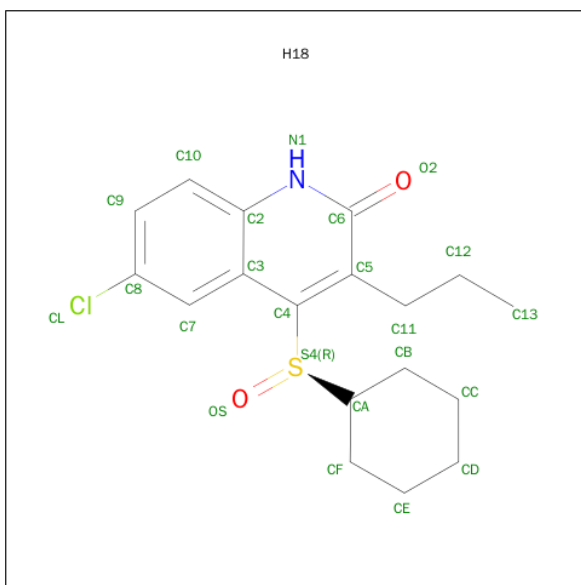
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	400	Total	C	N	O	S	0	0	0
			3319	2168	546	598	7			

- 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		
3	A	1	Total	O	P	0	0
			5	4	1		

- Molecule 4 is 6-CHLORO-4-(CYCLOHEXYLSULFINYL)-3-PROPYLQUINOLIN-2(1H)-ONE (three-letter code: H18) (formula: C<sub>18</sub>H<sub>22</sub>ClNO<sub>2</sub>S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	A	1	Total	C	Cl	N	O	S	0	0
			23	18	1	1	2	1		



V372	L228	L303	V372	V88	T165	K166	L229	L304	V89	T166	K167	W229	L228	V88
T375	W229	A304	T375	GLU	K166	I167	W230	A305	GLU	K167	L168	W231	L229	GLU
T376	M230	N306	T376	VAL	I167	L168	M231	E305	VAL	L168	E169	G231	W230	VAL
T377	G231	L310	T377	LEU	L168	E169	G232	N306	LEU	E169	P170	E232	M230	LEU
T378	E232	K311	T378	GLY	E169	P170	E233	L310	GLY	P170	F171	L234	E232	GLY
S379	L234	K312	S379	ILE	P171	L234	E234	K311	ILE	F171	A172	H235	L234	ILE
I380	H235	P313	I380	P95	A172	H235	P236	P313	P95	R173	K174	P237	H235	P95
W383	P236	G316	W383	P96	K173	P236	P237	G316	P96	Q174	N175	K238	P236	P96
G384	P237	V317	G384	P97	Q174	N175	K238	V317	P97	P176	G99	L100	P237	P97
K385	K238	Y318	K385	A98	P176	G99	L100	Y318	A98	D177	L100	K101	K238	A98
T386	L100	Y319	T386	G99	D177	L100	K101	Y319	G99	Q182	K103	I244	L100	G99
F389	K101	S322	F389	L100	Q182	K103	I244	S322	L100	M184	D185	D250	K101	L100
K390	I244	L325	K390	K104	M184	D185	D250	L325	K104	D186	L187	W252	I244	K104
I393	D250	E328	I393	T107	D186	L187	W252	E328	T107	Y188	V189	V254	D250	T107
Q394	W252	I329	Q394	V108	Y188	V189	V254	I329	V108	G190	S191	D182	W252	V108
K395	V254	K330	K395	G112	G190	S191	D182	K330	G112	T195	G196	V261	V254	G112
E396	D182	Q332	E396	Y115	T195	G196	V261	Q332	Y115	Q197	H198	L264	D182	Y115
W397	V261	G333	W397	F116	Q197	H198	L264	G333	F116	R199	E222	W265	V261	F116
T398	L264	Q334	T398	S117	R199	E222	W265	Q334	S117	T200	K201	W266	L264	S117
E399	W265	Q335	E399	V118	T200	K201	W266	Q335	V118	T202	E203	L274	W265	V118
W400	W266	G336	W400	P119	T202	E203	L274	G336	P119	L205	R206	K275	W266	P119
W401	L274	Q337	W401	E122	L205	R206	K275	Q337	E122	Q207	H208	Q278	L274	E122
Y405	K275	W337	Y405	R125	Q207	H208	Q278	W337	R125	L209	L210	K281	K275	R125
P413	Q278	T338	P413	T131	L209	L210	K281	T338	T131	R211	W212	L282	Q278	T131
W414	K281	Y339	W414	I135	R211	W212	L282	Y339	I135	G213	L214	R289	K281	I135
E415	L282	Q340	E415	N136	G213	L214	R289	Q340	N136	THR	THR	T290	L282	N136
F416	R289	I341	F416	E137	THR	THR	T290	I341	E137	PRO	PRO	L293	R289	E137
W417	T290	Y342	W417	E138	PRO	PRO	L293	Y342	E138	ASP	ASP	P294	T290	E138
N418	L293	F346	N418	E139	ASP	ASP	P294	F346	E139	LYS	LYS	L295	L293	E139
T419	P294	K347	T419	P140	LYS	LYS	L295	K347	P140	LYS	LYS	T296	P294	P140
P420	L295	N348	P420	B143	LYS	LYS	T296	N348	B143	GLN	GLN	E297	L295	B143
P421	T296	T351	P421	Y144	GLN	GLN	E297	T351	Y144	LYS	LYS	E298	T296	Y144
L422	E297	G352	L422	Q145	LYS	LYS	E298	G352	Q145	GLU	GLU	A299	E297	Q145
V423	E298	K353	V423	Y146	GLU	GLU	A299	K353	Y146	P225	P226	L301	E298	Y146
K424	A299	Y354	K424	P150	P225	P226	L301	Y354	P150	F160	S163	M164	A299	P150
L425	P225	A355	L425	Q151	F160	S163	M164	A355	Q151	G152	W153	K154	P225	Q151
W426	F160	R356	W426	G152	W153	K154	P157	R356	G152	K154	P157	F160	F160	G152
Y427	K154	MET	Y427	P157	K154	P157	F160	MET	P157	P157	F160	S163	S163	P157
Q428	P157	ARG	Q428	F160	S163	M164	F160	ARG	F160	S163	M164	F160	F160	S163
L429	S163	GLY	L429	S163	M164	F160	F160	GLY	S163	M164	F160	F160	S163	M164
E430	M164	ALA	E430	M164	F160	F160	F160	ALA	M164	F160	F160	F160	S163	M164
LYS	F160	HIS	LYS	F160	S163	M164	F160	HIS	F160	S163	M164	F160	S163	M164
GLU	S163	T362	GLU	S163	M164	F160	F160	T362	S163	M164	F160	F160	S163	M164
PRO	M164	N363	PRO	M164	F160	F160	F160	N363	M164	F160	F160	F160	S163	M164
ILE	F160	D364	ILE	F160	S163	M164	F160	D364	F160	S163	M164	F160	S163	M164
VAL	S163	V365	VAL	S163	M164	F160	F160	V365	S163	M164	F160	F160	S163	M164
GLY	M164	K366	GLY	M164	F160	F160	F160	K366	M164	F160	F160	F160	S163	M164
ALA	F160	Q367	ALA	F160	S163	M164	F160	Q367	F160	S163	M164	F160	S163	M164
GLU	F160	L368	GLU	F160	M164	F160	F160	L368	F160	M164	F160	F160	S163	M164
THR	S163	T369	THR	S163	M164	F160	F160	T369	S163	M164	F160	F160	S163	M164
PHE	M164	E370	PHE	M164	F160	F160	F160	E370	M164	F160	F160	F160	S163	M164

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	137.50 Å 115.30 Å 65.40 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	24.91 – 2.90 24.91 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.2 (24.91-2.90) 99.3 (24.91-2.90)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.25 (at 2.89 Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.221 , 0.281 0.217 , 0.234	Depositor DCC
$R_{free}$ test set	1135 reflections (4.82%)	DCC
Wilson B-factor (Å <sup>2</sup> )	71.7	Xtriage
Anisotropy	0.197	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 88.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 23552 reflections	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	7604	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.97% 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: H18, CSD, PO4

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	0.51	0/4352	0.72	0/5918
2	B	0.50	1/3415 (0.0%)	0.72	0/4639
All	All	0.51	1/7767 (0.0%)	0.72	0/10557

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	24	TRP	CB-CG	5.12	1.59	1.50

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	4247	0	4274	309	0
2	B	3319	0	3341	210	0
3	A	15	0	0	1	0
4	A	23	0	22	5	0
All	All	7604	0	7637	497	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 33.

All (497) 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:178:ILE:HD11	1:A:201:LYS:HG2	1.31	1.13
1:A:91:GLN:NE2	2:B:137:ASN:HB3	1.72	1.05
1:A:253:THR:HG22	1:A:255:ASN:H	1.17	1.02
2:B:261:VAL:HG13	2:B:276:VAL:HG11	1.43	1.00
2:B:63:ILE:HD11	2:B:72:ARG:HD3	1.44	0.99
2:B:227:PHE:HB3	2:B:231:GLY:HA2	1.46	0.95
2:B:332:GLN:HB3	2:B:428:GLN:NE2	1.80	0.95
2:B:266:TRP:O	2:B:269:GLN:HG2	1.69	0.92
1:A:91:GLN:HE21	2:B:137:ASN:HB3	1.34	0.88
2:B:169:GLU:O	2:B:173:LYS:HG3	1.75	0.85
1:A:70:LYS:HG3	1:A:71:TRP:H	1.38	0.85
1:A:253:THR:HG22	1:A:255:ASN:N	1.93	0.84
1:A:195:ILE:HD13	1:A:195:ILE:N	1.93	0.84
1:A:522:ILE:O	1:A:526:ILE:HG13	1.79	0.82
2:B:328:GLU:HG2	2:B:390:LYS:HD2	1.61	0.82
2:B:429:LEU:HD13	2:B:430:GLU:O	1.80	0.81
1:A:469:LEU:HD21	1:A:480:GLN:HG3	1.60	0.81
1:A:57:ASN:HA	1:A:129:ALA:O	1.79	0.81
1:A:225:PRO:HG2	1:A:236:PRO:HG3	1.60	0.81
2:B:332:GLN:HA	2:B:424:LYS:HE3	1.62	0.80
1:A:41:MET:HB2	1:A:47:ILE:HD11	1.64	0.80
1:A:206:ARG:HH22	1:A:218:ASP:HA	1.48	0.79
2:B:178:ILE:HD11	2:B:201:LYS:HG3	1.64	0.79
1:A:122:GLU:HA	1:A:125:ARG:HD2	1.63	0.79
1:A:319:TYR:OH	1:A:385:LYS:HE2	1.83	0.78
1:A:399:GLU:HG3	1:A:402:TRP:CE3	2.18	0.78
2:B:362:THR:HG22	2:B:366:LYS:HD3	1.65	0.78
2:B:295:LEU:HD12	2:B:295:LEU:H	1.49	0.77
1:A:122:GLU:HG3	1:A:125:ARG:NH1	1.99	0.77
2:B:420:PRO:O	2:B:423:VAL:HG12	1.86	0.76
1:A:28:GLU:OE1	1:A:135:ILE:HG22	1.86	0.75
1:A:178:ILE:CD1	1:A:201:LYS:HG2	2.12	0.74
1:A:107:THR:HG21	1:A:202:ILE:HG21	1.68	0.74
1:A:354:TYR:HD2	1:A:374:LYS:HD3	1.52	0.74
2:B:60:VAL:HG12	2:B:75:VAL:HG22	1.70	0.73
1:A:10:VAL:HG21	1:A:153:TRP:HH2	1.53	0.73
1:A:171:PHE:CE1	1:A:205:LEU:HA	2.24	0.73
1:A:412:PRO:HG3	2:B:401:TRP:HZ2	1.54	0.73
1:A:181:TYR:CE1	1:A:183:TYR:HB2	2.25	0.72
2:B:151:GLN:HB3	2:B:185:ASP:OD1	1.89	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:198:HIS:O	1:A:202:ILE:HG12	1.89	0.72
2:B:241:VAL:HG11	2:B:313:PRO:HG3	1.70	0.72
2:B:104:LYS:HB2	2:B:192:ASP:HA	1.71	0.72
2:B:201:LYS:HA	2:B:201:LYS:HE3	1.70	0.72
2:B:295:LEU:HD12	2:B:295:LEU:N	2.05	0.71
2:B:332:GLN:HG3	2:B:338:THR:HG23	1.72	0.70
1:A:500:GLN:HE21	2:B:422:LEU:HD12	1.56	0.70
2:B:169:GLU:N	2:B:170:PRO:HD2	2.06	0.70
1:A:343:GLN:HG3	1:A:349:LEU:HD11	1.72	0.70
1:A:500:GLN:NE2	2:B:422:LEU:HD12	2.08	0.69
1:A:435:VAL:HG22	2:B:290:THR:HG21	1.72	0.69
2:B:169:GLU:HG2	2:B:170:PRO:HD3	1.74	0.69
1:A:442:VAL:HB	1:A:481:ALA:HB1	1.74	0.69
1:A:342:TYR:HA	1:A:349:LEU:HD12	1.74	0.69
2:B:236:PRO:HA	2:B:239:TRP:CE2	2.27	0.69
1:A:102:LYS:HG3	1:A:237:ASP:HA	1.75	0.69
1:A:206:ARG:NH2	1:A:218:ASP:HA	2.08	0.68
1:A:206:ARG:CZ	1:A:217:PRO:O	2.42	0.68
1:A:79:GLU:OE2	1:A:83:ARG:NH1	2.26	0.68
1:A:412:PRO:HG3	2:B:401:TRP:CZ2	2.29	0.68
2:B:203:GLU:HG3	2:B:207:GLN:HE22	1.58	0.67
1:A:317:VAL:HG22	1:A:318:TYR:N	2.09	0.67
1:A:480:GLN:HG2	1:A:517:LEU:HD11	1.76	0.67
2:B:28:GLU:HB2	2:B:135:ILE:HD11	1.75	0.67
1:A:177:ASP:OD2	1:A:193:LEU:HD21	1.94	0.67
1:A:417:VAL:O	1:A:417:VAL:HG13	1.95	0.66
2:B:236:PRO:HA	2:B:239:TRP:CD2	2.30	0.66
1:A:503:LEU:HD12	1:A:533:LEU:HD23	1.78	0.66
1:A:174:GLN:C	1:A:176:PRO:HD3	2.15	0.66
1:A:164:MET:O	1:A:168:LEU:HG	1.96	0.65
1:A:208:HIS:O	1:A:208:HIS:HD2	1.79	0.65
1:A:186:ASP:HB3	1:A:188:TYR:CE1	2.31	0.65
1:A:174:GLN:HE21	1:A:174:GLN:HA	1.61	0.65
1:A:54:ASN:ND2	1:A:126:LYS:HB2	2.12	0.65
1:A:72:ARG:HG2	1:A:73:LYS:N	2.11	0.65
2:B:242:GLN:HG2	2:B:353:LYS:HE3	1.78	0.65
2:B:202:ILE:HG21	2:B:227:PHE:HE1	1.61	0.64
2:B:227:PHE:HB3	2:B:231:GLY:CA	2.26	0.64
2:B:203:GLU:HG3	2:B:207:GLN:NE2	2.12	0.64
1:A:92:LEU:O	1:A:92:LEU:HD23	1.97	0.64
2:B:175:ASN:HD21	2:B:201:LYS:NZ	1.96	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:104:LYS:HD2	2:B:192:ASP:O	1.97	0.64
1:A:20:LYS:HD2	1:A:55:PRO:HB2	1.78	0.64
2:B:298:GLU:CD	2:B:298:GLU:H	2.01	0.64
1:A:107:THR:HB	1:A:202:ILE:HD12	1.79	0.64
1:A:108:VAL:HG13	1:A:223:LYS:HB2	1.80	0.64
2:B:27:THR:OG1	2:B:30:LYS:HG2	1.98	0.64
1:A:500:GLN:HE21	2:B:422:LEU:CD1	2.10	0.64
1:A:31:ILE:O	1:A:35:VAL:HG23	1.98	0.63
1:A:472:THR:OG1	1:A:476:LYS:HE3	1.98	0.63
2:B:173:LYS:O	2:B:176:PRO:HD3	1.99	0.63
1:A:363:ASN:ND2	1:A:401:TRP:CZ3	2.67	0.63
2:B:366:LYS:HG3	2:B:405:TYR:CD2	2.34	0.62
1:A:317:VAL:HG22	1:A:318:TYR:H	1.64	0.62
1:A:96:HIS:H	2:B:136:ASN:HD21	1.47	0.62
1:A:41:MET:HB2	1:A:47:ILE:CD1	2.28	0.62
1:A:86:ASP:HA	1:A:154:LYS:HZ1	1.65	0.62
1:A:238:LYS:HD2	1:A:315:HIS:CG	2.33	0.62
1:A:13:LYS:HE3	1:A:84:THR:O	1.99	0.62
2:B:365:VAL:HG11	2:B:401:TRP:HB2	1.80	0.62
1:A:195:ILE:CD1	1:A:195:ILE:N	2.63	0.62
1:A:475:GLN:HB3	1:A:501:TYR:CE2	2.34	0.62
1:A:12:LEU:HD11	1:A:127:TYR:CE1	2.34	0.62
1:A:279:LEU:HD23	1:A:282:LEU:HD11	1.82	0.62
1:A:523:GLU:O	1:A:527:LYS:HG2	1.99	0.61
1:A:174:GLN:NE2	1:A:174:GLN:HA	2.15	0.61
2:B:234:LEU:HD21	2:B:377:THR:CG2	2.30	0.61
1:A:417:VAL:O	1:A:419:THR:N	2.33	0.61
1:A:460:ASN:ND2	3:A:1301:PO4:O4	2.33	0.61
1:A:368:LEU:O	1:A:372:VAL:HG23	2.01	0.61
1:A:12:LEU:HD11	1:A:127:TYR:CZ	2.36	0.61
2:B:167:ILE:O	2:B:208:HIS:HE1	1.82	0.61
2:B:395:LYS:HG3	2:B:416:PHE:CE1	2.36	0.61
1:A:91:GLN:C	1:A:93:GLY:H	2.05	0.60
2:B:203:GLU:CG	2:B:207:GLN:HE22	2.14	0.60
2:B:241:VAL:O	2:B:243:PRO:HD3	2.02	0.60
2:B:115:TYR:C	2:B:117:SER:H	2.05	0.60
2:B:85:GLN:O	2:B:85:GLN:HG3	2.01	0.60
1:A:507:GLN:HE22	2:B:421:PRO:HB3	1.67	0.60
1:A:476:LYS:HD2	1:A:476:LYS:O	2.02	0.60
1:A:171:PHE:HB2	1:A:208:HIS:CE1	2.37	0.60
1:A:292:VAL:C	1:A:293:ILE:HD12	2.21	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:101:LYS:N	1:A:101:LYS:HD2	2.16	0.59
1:A:403:THR:CG2	2:B:334:GLN:H	2.14	0.59
1:A:354:TYR:CD2	1:A:374:LYS:HD3	2.37	0.59
1:A:229:TRP:CE2	4:A:999:H18:HD1	2.37	0.59
1:A:399:GLU:HG3	1:A:402:TRP:CZ3	2.37	0.59
1:A:85:GLN:C	1:A:154:LYS:HZ3	2.06	0.59
1:A:411:ILE:O	1:A:412:PRO:O	2.20	0.59
2:B:395:LYS:NZ	2:B:399:GLU:HG3	2.17	0.59
2:B:139:THR:HB	2:B:140:PRO:HD2	1.84	0.59
2:B:365:VAL:O	2:B:369:THR:HG23	2.03	0.58
1:A:89:GLU:OE1	1:A:89:GLU:HA	2.03	0.58
1:A:10:VAL:HG12	1:A:11:LYS:N	2.18	0.58
1:A:172:ARG:NH1	1:A:180:ILE:HB	2.18	0.58
2:B:298:GLU:N	2:B:298:GLU:OE1	2.35	0.58
2:B:261:VAL:HG13	2:B:276:VAL:CG1	2.24	0.58
2:B:295:LEU:H	2:B:295:LEU:CD1	2.15	0.58
2:B:170:PRO:HA	2:B:173:LYS:NZ	2.19	0.58
2:B:28:GLU:CB	2:B:135:ILE:HD11	2.34	0.57
2:B:205:LEU:O	2:B:209:LEU:HG	2.03	0.57
2:B:274:ILE:HD11	2:B:310:LEU:HD21	1.85	0.57
1:A:233:GLU:HB3	1:A:240:THR:HG23	1.86	0.57
2:B:168:LEU:C	2:B:170:PRO:HD2	2.24	0.57
2:B:234:LEU:HD21	2:B:377:THR:HG21	1.87	0.57
1:A:491:LEU:HD23	1:A:529:GLU:CG	2.34	0.57
1:A:330:GLN:NE2	1:A:340:GLN:OE1	2.34	0.57
1:A:58:THR:HG23	1:A:76:ASP:O	2.04	0.57
2:B:195:ILE:HG13	2:B:199:ARG:HE	1.69	0.57
1:A:34:LEU:HD13	1:A:132:ILE:HD12	1.86	0.57
1:A:181:TYR:HH	1:A:183:TYR:HD2	1.53	0.57
1:A:329:ILE:HD11	1:A:375:ILE:HD12	1.87	0.57
2:B:282:LEU:HD21	2:B:296:THR:HG23	1.86	0.57
1:A:195:ILE:H	1:A:195:ILE:HD13	1.70	0.57
1:A:208:HIS:O	1:A:208:HIS:CD2	2.57	0.56
2:B:115:TYR:O	2:B:117:SER:N	2.37	0.56
1:A:107:THR:HG23	1:A:222:GLN:NE2	2.19	0.56
1:A:131:THR:HG23	1:A:143:ARG:HG2	1.86	0.56
1:A:231:GLY:O	1:A:266:TRP:HZ2	1.88	0.56
2:B:38:CYS:SG	2:B:73:LYS:HE2	2.46	0.56
2:B:58:THR:HG21	2:B:77:PHE:CD2	2.39	0.56
1:A:125:ARG:HG2	1:A:146:TYR:O	2.06	0.56
2:B:167:ILE:O	2:B:208:HIS:CE1	2.58	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:62:ALA:C	1:A:63:ILE:HD12	2.26	0.56
1:A:491:LEU:HD23	1:A:529:GLU:HG2	1.86	0.56
1:A:91:GLN:O	1:A:93:GLY:N	2.39	0.56
2:B:257:ILE:HG21	2:B:283:LEU:HD13	1.89	0.55
2:B:332:GLN:CG	2:B:338:THR:HG23	2.37	0.55
2:B:31:ILE:O	2:B:35:VAL:HG23	2.06	0.55
1:A:116:PHE:CD2	1:A:116:PHE:N	2.74	0.55
1:A:440:PHE:HZ	1:A:463:ARG:HH21	1.53	0.55
1:A:206:ARG:HH12	1:A:218:ASP:HA	1.71	0.55
1:A:376:THR:HG23	1:A:386:THR:HG22	1.89	0.55
2:B:175:ASN:HD21	2:B:201:LYS:HZ2	1.54	0.55
2:B:170:PRO:HG2	2:B:171:PHE:H	1.71	0.55
2:B:183:TYR:OH	2:B:386:THR:HG23	2.07	0.55
1:A:27:THR:HG23	1:A:30:LYS:HB2	1.88	0.55
2:B:414:TRP:O	2:B:414:TRP:HD1	1.90	0.55
2:B:380:ILE:O	2:B:384:GLY:N	2.34	0.55
2:B:254:VAL:O	2:B:258:GLN:HG3	2.07	0.55
2:B:116:PHE:CE1	2:B:151:GLN:HG3	2.42	0.55
1:A:114:ALA:HB1	1:A:160:PHE:CE2	2.42	0.55
1:A:219:LYS:HD2	1:A:222:GLN:NE2	2.23	0.54
1:A:348:ASN:ND2	1:A:351:THR:CG2	2.71	0.54
2:B:169:GLU:HG2	2:B:170:PRO:CD	2.38	0.54
2:B:178:ILE:CD1	2:B:201:LYS:HD2	2.37	0.54
2:B:175:ASN:ND2	2:B:201:LYS:NZ	2.54	0.54
1:A:208:HIS:C	1:A:208:HIS:CD2	2.80	0.54
1:A:296:THR:HG22	1:A:297:GLU:N	2.21	0.54
1:A:58:THR:CG2	1:A:76:ASP:O	2.56	0.54
1:A:96:HIS:H	2:B:136:ASN:ND2	2.05	0.54
1:A:380:ILE:HD13	2:B:27:THR:HG22	1.90	0.54
1:A:61:PHE:CE1	1:A:63:ILE:HD11	2.43	0.54
1:A:171:PHE:HB2	1:A:208:HIS:ND1	2.23	0.54
1:A:340:GLN:HB3	1:A:351:THR:HG22	1.89	0.54
1:A:470:THR:O	1:A:471:ASP:HB2	2.08	0.54
2:B:227:PHE:CB	2:B:231:GLY:HA2	2.30	0.54
2:B:335:GLY:O	2:B:355:ALA:HA	2.08	0.54
1:A:340:GLN:CB	1:A:351:THR:HG22	2.37	0.53
1:A:358:ARG:HD3	1:A:370:GLU:CD	2.29	0.53
1:A:253:THR:CG2	1:A:254:VAL:N	2.70	0.53
2:B:277:ARG:O	2:B:281:LYS:HG3	2.08	0.53
2:B:201:LYS:HD3	2:B:201:LYS:O	2.08	0.53
1:A:26:LEU:HD12	1:A:133:PRO:CD	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:376:THR:HG23	1:A:386:THR:CG2	2.39	0.53
1:A:40:GLU:HA	1:A:40:GLU:OE2	2.08	0.53
2:B:175:ASN:N	2:B:176:PRO:HD3	2.22	0.53
1:A:29:GLU:HG2	1:A:29:GLU:O	2.09	0.53
1:A:115:TYR:O	1:A:149:LEU:HB2	2.09	0.53
2:B:203:GLU:OE2	2:B:207:GLN:NE2	2.40	0.53
1:A:358:ARG:NH2	2:B:394:GLN:HG2	2.24	0.53
1:A:476:LYS:HD3	1:A:517:LEU:HD12	1.90	0.52
2:B:425:LEU:HD23	2:B:425:LEU:O	2.09	0.52
1:A:70:LYS:HG3	1:A:71:TRP:N	2.16	0.52
1:A:56:TYR:O	1:A:143:ARG:NH2	2.35	0.52
1:A:194:GLU:O	1:A:196:GLY:N	2.42	0.52
2:B:203:GLU:CD	2:B:207:GLN:HE22	2.11	0.52
2:B:342:TYR:HB3	2:B:348:ASN:HA	1.90	0.52
2:B:330:GLN:HB2	2:B:338:THR:OG1	2.09	0.52
1:A:469:LEU:HD21	1:A:480:GLN:CG	2.35	0.52
2:B:79:GLU:O	2:B:83:ARG:HG3	2.09	0.52
1:A:236:PRO:HA	4:A:999:H18:H9	1.92	0.52
2:B:175:ASN:O	2:B:178:ILE:HB	2.10	0.52
1:A:206:ARG:NH1	1:A:218:ASP:HA	2.25	0.52
1:A:268:SER:OG	1:A:353:LYS:HE2	2.09	0.52
1:A:498:ASP:O	1:A:535:TRP:NE1	2.41	0.51
1:A:507:GLN:NE2	2:B:421:PRO:HB3	2.25	0.51
1:A:86:ASP:HA	1:A:154:LYS:NZ	2.24	0.51
1:A:108:VAL:CG1	1:A:223:LYS:HB2	2.40	0.51
2:B:297:GLU:HA	2:B:300:GLU:HB2	1.91	0.51
2:B:146:TYR:CD2	2:B:150:PRO:HB3	2.45	0.51
2:B:125:ARG:HB3	2:B:145:GLN:HE21	1.75	0.51
1:A:382:ILE:O	2:B:136:ASN:HB2	2.11	0.51
2:B:7:THR:HG22	2:B:119:PRO:HG2	1.92	0.51
2:B:264:LEU:HD13	2:B:306:ASN:HD22	1.75	0.51
1:A:515:SER:O	1:A:519:ASN:ND2	2.42	0.51
2:B:115:TYR:OH	2:B:157:PRO:HG3	2.11	0.51
1:A:225:PRO:HB3	1:A:236:PRO:HD3	1.92	0.51
2:B:366:LYS:O	2:B:370:GLU:HG3	2.11	0.51
1:A:164:MET:HE1	1:A:168:LEU:HD21	1.92	0.51
2:B:306:ASN:O	2:B:310:LEU:HG	2.11	0.51
2:B:282:LEU:HB3	2:B:293:ILE:HG21	1.93	0.50
2:B:57:ASN:ND2	2:B:131:THR:OG1	2.43	0.50
1:A:408:ALA:HB1	2:B:364:ASP:HB3	1.93	0.50
1:A:19:PRO:HD3	1:A:80:LEU:HD13	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:406:TRP:HH2	2:B:418:ASN:OD1	1.94	0.50
1:A:328:GLU:O	1:A:339:TYR:HA	2.10	0.50
1:A:169:GLU:HB3	1:A:170:PRO:HD3	1.94	0.50
1:A:70:LYS:CG	1:A:71:TRP:H	2.17	0.50
2:B:146:TYR:CG	2:B:150:PRO:HB3	2.47	0.50
2:B:372:VAL:HG13	2:B:389:PHE:CZ	2.47	0.50
2:B:107:THR:HB	2:B:202:ILE:HD11	1.94	0.50
1:A:399:GLU:HA	1:A:402:TRP:HE3	1.76	0.50
1:A:393:ILE:HD12	1:A:423:VAL:HG21	1.93	0.50
1:A:260:LEU:HD23	1:A:279:LEU:HD13	1.94	0.50
2:B:393:ILE:HD11	2:B:397:THR:HG22	1.94	0.50
1:A:111:VAL:CG1	1:A:114:ALA:HB2	2.41	0.49
1:A:476:LYS:CD	1:A:517:LEU:HD12	2.41	0.49
1:A:188:TYR:CD2	4:A:999:H18:HF1	2.47	0.49
1:A:319:TYR:O	1:A:321:PRO:HD3	2.12	0.49
2:B:28:GLU:HB2	2:B:135:ILE:CD1	2.42	0.49
2:B:175:ASN:ND2	2:B:201:LYS:HZ2	2.10	0.49
1:A:175:ASN:N	1:A:176:PRO:HD3	2.26	0.49
1:A:278:GLN:HA	1:A:278:GLN:NE2	2.27	0.49
1:A:207:GLN:NE2	1:A:210:LEU:HD12	2.27	0.49
2:B:239:TRP:CH2	2:B:378:GLU:HG2	2.47	0.49
1:A:54:ASN:O	1:A:143:ARG:NH2	2.43	0.49
2:B:331:LYS:HB2	2:B:337:TRP:CZ3	2.47	0.49
2:B:244:ILE:HD13	2:B:266:TRP:CZ3	2.48	0.49
2:B:125:ARG:HB3	2:B:145:GLN:NE2	2.28	0.49
1:A:210:LEU:C	1:A:212:TRP:H	2.15	0.49
2:B:178:ILE:HD11	2:B:201:LYS:CG	2.40	0.49
2:B:328:GLU:CG	2:B:390:LYS:HD2	2.36	0.49
1:A:10:VAL:O	1:A:11:LYS:HG3	2.13	0.49
2:B:372:VAL:HG13	2:B:389:PHE:CE2	2.48	0.49
2:B:423:VAL:O	2:B:427:TYR:HD2	1.96	0.49
1:A:229:TRP:O	1:A:232:TYR:HB2	2.13	0.49
2:B:278:GLN:NE2	2:B:298:GLU:HB2	2.28	0.49
1:A:277:ARG:HH11	1:A:277:ARG:HG3	1.78	0.49
2:B:295:LEU:CD1	2:B:295:LEU:N	2.75	0.48
2:B:170:PRO:HA	2:B:173:LYS:HZ3	1.77	0.48
1:A:108:VAL:HG12	1:A:223:LYS:O	2.13	0.48
1:A:63:ILE:N	1:A:63:ILE:HD12	2.28	0.48
1:A:181:TYR:OH	1:A:183:TYR:HD2	1.95	0.48
2:B:136:ASN:O	2:B:138:GLU:HG3	2.14	0.48
2:B:178:ILE:HD12	2:B:201:LYS:HD2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:10:VAL:HG21	1:A:153:TRP:CH2	2.43	0.48
1:A:500:GLN:O	1:A:503:LEU:HB3	2.12	0.48
1:A:399:GLU:HG3	1:A:402:TRP:HE3	1.75	0.48
1:A:131:THR:OG1	1:A:143:ARG:CD	2.62	0.48
2:B:319:TYR:HE2	2:B:325:LEU:HD13	1.78	0.48
2:B:208:HIS:HA	2:B:211:ARG:HD3	1.95	0.48
1:A:50:ILE:HD12	1:A:54:ASN:HB3	1.96	0.48
1:A:145:GLN:O	1:A:145:GLN:HG3	2.14	0.48
1:A:86:ASP:CA	1:A:154:LYS:HZ1	2.25	0.48
1:A:293:ILE:HD12	1:A:293:ILE:N	2.29	0.47
1:A:231:GLY:O	1:A:266:TRP:CZ2	2.67	0.47
2:B:368:LEU:O	2:B:372:VAL:HG23	2.14	0.47
1:A:23:GLN:NE2	1:A:26:LEU:HG	2.28	0.47
1:A:38:CYS:SG	1:A:73:LYS:HE3	2.54	0.47
1:A:107:THR:HG21	1:A:202:ILE:CG2	2.41	0.47
1:A:255:ASN:HB2	1:A:289:LEU:O	2.15	0.47
1:A:241:VAL:HG22	1:A:270:ILE:HG21	1.95	0.47
2:B:10:VAL:HG21	2:B:153:TRP:HH2	1.79	0.47
1:A:254:VAL:CG2	1:A:293:ILE:HD11	2.45	0.47
1:A:518:VAL:O	1:A:522:ILE:HG13	2.15	0.47
1:A:469:LEU:CD2	1:A:480:GLN:HG3	2.40	0.47
1:A:225:PRO:CB	1:A:236:PRO:HD3	2.44	0.47
1:A:130:PHE:CE2	1:A:144:TYR:HB2	2.50	0.47
2:B:99:GLY:HA2	2:B:102:LYS:HE2	1.96	0.47
2:B:369:THR:HG22	2:B:398:TRP:CZ3	2.49	0.47
2:B:57:ASN:HD22	2:B:143:ARG:NH1	2.12	0.47
2:B:97:PRO:C	2:B:99:GLY:N	2.66	0.47
1:A:136:ASN:OD1	1:A:139:THR:HG23	2.14	0.47
2:B:108:VAL:HG12	2:B:228:LEU:HD12	1.96	0.47
2:B:379:SER:HA	2:B:383:TRP:CE3	2.50	0.47
2:B:21:VAL:HB	2:B:59:PRO:HD3	1.97	0.46
1:A:346:PHE:CD1	1:A:346:PHE:N	2.82	0.46
2:B:189:VAL:HG11	2:B:202:ILE:HD13	1.97	0.46
2:B:332:GLN:OE1	2:B:428:GLN:CD	2.53	0.46
1:A:340:GLN:HA	1:A:351:THR:HA	1.96	0.46
1:A:238:LYS:NZ	1:A:315:HIS:CD2	2.83	0.46
2:B:169:GLU:N	2:B:170:PRO:CD	2.76	0.46
1:A:164:MET:CE	1:A:168:LEU:HD11	2.45	0.46
2:B:195:ILE:HG23	2:B:196:GLY:N	2.31	0.46
1:A:24:TRP:CZ3	1:A:61:PHE:HB3	2.51	0.46
1:A:393:ILE:HB	1:A:423:VAL:HG22	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:97:PRO:C	2:B:99:GLY:H	2.18	0.46
1:A:348:ASN:ND2	1:A:351:THR:HG21	2.31	0.46
2:B:348:ASN:HD22	2:B:351:THR:CG2	2.29	0.46
1:A:224:GLU:HB3	1:A:225:PRO:HD2	1.96	0.46
2:B:24:TRP:CD1	2:B:25:PRO:HD2	2.51	0.46
1:A:117:SER:OG	1:A:214:LEU:HD23	2.16	0.46
2:B:393:ILE:HD11	2:B:397:THR:CG2	2.46	0.46
1:A:408:ALA:HB2	2:B:337:TRP:HH2	1.80	0.46
2:B:174:GLN:C	2:B:176:PRO:HD3	2.36	0.46
1:A:417:VAL:O	1:A:417:VAL:CG1	2.61	0.46
2:B:195:ILE:CG2	2:B:196:GLY:N	2.79	0.46
1:A:486:LEU:HD13	1:A:524:GLN:HB2	1.98	0.46
1:A:270:ILE:HG13	1:A:314:VAL:HG23	1.98	0.45
1:A:183:TYR:O	1:A:184:MET:HB2	2.17	0.45
1:A:206:ARG:CZ	1:A:218:ASP:HA	2.45	0.45
1:A:317:VAL:CG2	1:A:318:TYR:N	2.76	0.45
1:A:238:LYS:HD2	1:A:315:HIS:CD2	2.51	0.45
2:B:40:GLU:HG3	2:B:44:GLU:OE2	2.16	0.45
1:A:283:LEU:O	1:A:286:THR:HG23	2.15	0.45
1:A:235:HIS:O	4:A:999:H18:H9	2.16	0.45
1:A:501:TYR:CE1	1:A:505:ILE:HD11	2.51	0.45
1:A:28:GLU:OE1	1:A:135:ILE:CG2	2.61	0.45
1:A:18:GLY:HA3	1:A:56:TYR:CE1	2.52	0.45
1:A:363:ASN:ND2	1:A:401:TRP:CH2	2.84	0.45
1:A:306:ASN:O	1:A:310:LEU:HG	2.15	0.45
1:A:18:GLY:HA3	1:A:56:TYR:CD1	2.52	0.45
1:A:27:THR:O	1:A:30:LYS:N	2.48	0.45
1:A:53:GLU:O	1:A:55:PRO:HD3	2.16	0.45
1:A:401:TRP:HH2	1:A:508:ALA:O	2.00	0.45
1:A:482:ILE:HD12	1:A:502:ALA:HB1	1.99	0.45
1:A:27:THR:HG23	1:A:30:LYS:CB	2.46	0.45
1:A:95:PRO:HG3	2:B:137:ASN:O	2.17	0.44
4:A:999:H18:H7	4:A:999:H18:OS	2.17	0.44
2:B:264:LEU:HD13	2:B:306:ASN:ND2	2.32	0.44
2:B:108:VAL:HG22	2:B:188:TYR:CD2	2.52	0.44
2:B:208:HIS:ND1	2:B:208:HIS:O	2.50	0.44
1:A:395:LYS:O	1:A:399:GLU:HB2	2.17	0.44
1:A:240:THR:OG1	1:A:241:VAL:N	2.50	0.44
1:A:40:GLU:CA	1:A:40:GLU:OE2	2.65	0.44
1:A:222:GLN:HB3	1:A:223:LYS:H	1.69	0.44
2:B:182:GLN:HB2	2:B:187:LEU:CD1	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:410:TRP:CE3	2:B:363:ASN:HB2	2.53	0.44
1:A:324:ASP:O	1:A:343:GLN:HG2	2.17	0.44
2:B:234:LEU:HD12	2:B:234:LEU:N	2.32	0.44
1:A:142:ILE:HD12	1:A:144:TYR:OH	2.17	0.44
2:B:278:GLN:HB3	2:B:299:ALA:HA	2.00	0.44
2:B:369:THR:HG22	2:B:398:TRP:CH2	2.52	0.44
1:A:34:LEU:HD13	1:A:132:ILE:CD1	2.47	0.44
2:B:429:LEU:CD1	2:B:430:GLU:N	2.81	0.44
1:A:48:SER:O	1:A:50:ILE:HG23	2.16	0.44
2:B:414:TRP:O	2:B:414:TRP:CD1	2.71	0.44
1:A:393:ILE:HB	1:A:423:VAL:CG2	2.48	0.44
1:A:332:GLN:HB3	1:A:336:GLN:HB3	2.00	0.44
2:B:339:TYR:CD1	2:B:375:ILE:HD11	2.53	0.44
2:B:154:LYS:O	2:B:157:PRO:HD2	2.18	0.43
1:A:74:LEU:C	1:A:74:LEU:HD12	2.38	0.43
1:A:406:TRP:CH2	2:B:418:ASN:HA	2.53	0.43
2:B:118:VAL:HG21	2:B:160:PHE:HD2	1.83	0.43
1:A:95:PRO:HG2	1:A:181:TYR:CE2	2.53	0.43
1:A:237:ASP:N	1:A:237:ASP:OD2	2.44	0.43
2:B:163:SER:O	2:B:167:ILE:HG13	2.18	0.43
1:A:164:MET:HE1	1:A:187:LEU:HD21	2.00	0.43
1:A:194:GLU:O	1:A:195:ILE:C	2.57	0.43
1:A:317:VAL:CG2	1:A:318:TYR:H	2.28	0.43
1:A:401:TRP:CH2	1:A:508:ALA:O	2.71	0.43
2:B:264:LEU:CD1	2:B:306:ASN:HD22	2.32	0.43
1:A:296:THR:CG2	1:A:297:GLU:N	2.81	0.43
2:B:228:LEU:HD23	2:B:228:LEU:HA	1.91	0.43
1:A:360:ALA:HB1	1:A:514:GLU:OE1	2.18	0.43
1:A:326:ILE:O	1:A:341:ILE:HA	2.19	0.43
1:A:253:THR:CG2	1:A:255:ASN:H	2.07	0.43
1:A:218:ASP:O	1:A:222:GLN:HG3	2.18	0.43
2:B:100:LEU:HD12	2:B:100:LEU:O	2.19	0.43
2:B:201:LYS:HD3	2:B:201:LYS:C	2.38	0.43
1:A:472:THR:CB	1:A:476:LYS:HE3	2.48	0.43
1:A:79:GLU:O	1:A:83:ARG:HG3	2.17	0.43
1:A:245:VAL:HG23	1:A:245:VAL:O	2.18	0.43
1:A:420:PRO:HA	1:A:421:PRO:C	2.39	0.43
1:A:131:THR:OG1	1:A:143:ARG:HD3	2.18	0.43
2:B:229:TRP:CE3	2:B:229:TRP:HA	2.53	0.43
1:A:111:VAL:HG12	1:A:114:ALA:HB2	1.99	0.43
2:B:150:PRO:HG2	2:B:153:TRP:HB2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:253:THR:CG2	1:A:289:LEU:O	2.67	0.43
1:A:210:LEU:C	1:A:212:TRP:N	2.71	0.43
2:B:230:MET:C	2:B:232:TYR:N	2.72	0.43
1:A:174:GLN:HE21	1:A:174:GLN:CA	2.27	0.43
1:A:226:PRO:HB3	1:A:235:HIS:CE1	2.54	0.43
2:B:50:ILE:CG2	2:B:145:GLN:HG2	2.49	0.43
1:A:277:ARG:NH1	1:A:277:ARG:HG3	2.33	0.43
1:A:177:ASP:OD1	1:A:177:ASP:N	2.48	0.42
1:A:520:GLN:HE21	1:A:520:GLN:HB2	1.57	0.42
2:B:98:ALA:O	2:B:101:LYS:HE3	2.19	0.42
1:A:206:ARG:HH12	1:A:219:LYS:N	2.17	0.42
2:B:112:GLY:HA3	2:B:151:GLN:OE1	2.18	0.42
1:A:23:GLN:NE2	1:A:24:TRP:O	2.41	0.42
1:A:296:THR:HG22	1:A:298:GLU:H	1.85	0.42
1:A:265:ASN:N	1:A:265:ASN:HD22	2.17	0.42
1:A:224:GLU:HB3	1:A:225:PRO:CD	2.49	0.42
2:B:376:THR:O	2:B:377:THR:C	2.57	0.42
1:A:433:PRO:HB3	2:B:289:LEU:HD23	2.01	0.42
1:A:239:TRP:NE1	1:A:316:GLY:HA3	2.35	0.42
2:B:316:GLY:HA2	2:B:318:TYR:CE2	2.54	0.42
1:A:91:GLN:C	1:A:93:GLY:N	2.71	0.42
2:B:104:LYS:CB	2:B:192:ASP:HA	2.46	0.42
2:B:378:GLU:O	2:B:379:SER:C	2.58	0.42
2:B:208:HIS:CG	2:B:208:HIS:O	2.72	0.42
2:B:355:ALA:O	2:B:356:ARG:C	2.57	0.42
1:A:283:LEU:C	1:A:286:THR:HG23	2.40	0.42
2:B:182:GLN:HA	2:B:187:LEU:HD12	2.01	0.42
2:B:252:TRP:CZ3	2:B:260:LEU:HD22	2.54	0.42
1:A:503:LEU:HD22	1:A:535:TRP:HB2	2.01	0.42
1:A:131:THR:OG1	1:A:143:ARG:HD2	2.19	0.42
2:B:98:ALA:O	2:B:101:LYS:HG2	2.19	0.42
2:B:301:LEU:O	2:B:304:ALA:HB3	2.19	0.42
2:B:160:PHE:CD1	2:B:160:PHE:O	2.73	0.42
1:A:207:GLN:CD	1:A:210:LEU:HD12	2.40	0.42
1:A:233:GLU:HB3	1:A:240:THR:CG2	2.48	0.41
1:A:63:ILE:HD13	1:A:74:LEU:HB3	2.00	0.41
1:A:96:HIS:HA	1:A:97:PRO:HD2	1.83	0.41
1:A:257:ILE:HD13	1:A:282:LEU:HD13	2.02	0.41
2:B:429:LEU:HB2	2:B:430:GLU:H	1.38	0.41
1:A:174:GLN:O	1:A:176:PRO:HD3	2.20	0.41
1:A:324:ASP:CG	1:A:388:LYS:HE3	2.40	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:391:LEU:HB2	1:A:393:ILE:HG22	2.02	0.41
1:A:486:LEU:CD1	1:A:521:ILE:HG23	2.50	0.41
1:A:156:SER:N	1:A:157:PRO:CD	2.83	0.41
2:B:173:LYS:O	2:B:176:PRO:CD	2.66	0.41
1:A:10:VAL:CG1	1:A:11:LYS:N	2.82	0.41
1:A:115:TYR:N	1:A:115:TYR:CD2	2.89	0.41
2:B:136:ASN:O	2:B:137:ASN:C	2.58	0.41
1:A:116:PHE:H	1:A:116:PHE:HD2	1.68	0.41
1:A:282:LEU:HB3	1:A:293:ILE:HG21	2.02	0.41
1:A:160:PHE:CE2	1:A:164:MET:HG2	2.55	0.41
1:A:457:TYR:C	1:A:457:TYR:CD1	2.94	0.41
1:A:324:ASP:O	1:A:343:GLN:HA	2.20	0.41
1:A:23:GLN:HE21	1:A:26:LEU:HG	1.86	0.41
2:B:393:ILE:HG12	2:B:394:GLN:N	2.36	0.41
1:A:253:THR:HG22	1:A:254:VAL:N	2.36	0.41
1:A:54:ASN:HD21	1:A:126:LYS:HB2	1.84	0.41
1:A:130:PHE:CZ	1:A:144:TYR:HB2	2.56	0.41
2:B:259:LYS:HE2	2:B:259:LYS:HB3	1.82	0.41
1:A:175:ASN:OD1	1:A:201:LYS:HE2	2.20	0.41
2:B:429:LEU:HD13	2:B:430:GLU:N	2.36	0.41
1:A:226:PRO:HB3	1:A:235:HIS:ND1	2.36	0.41
1:A:116:PHE:HD2	1:A:116:PHE:N	2.19	0.41
1:A:440:PHE:CD2	1:A:459:THR:HG22	2.56	0.41
1:A:396:GLU:HG3	1:A:397:THR:N	2.36	0.41
2:B:338:THR:HG21	2:B:427:TYR:O	2.20	0.41
1:A:354:TYR:HD2	1:A:374:LYS:CD	2.26	0.41
1:A:362:THR:OG1	1:A:363:ASN:N	2.54	0.41
2:B:340:GLN:CG	2:B:351:THR:HG22	2.51	0.41
1:A:33:ALA:O	1:A:37:ILE:HG13	2.21	0.41
1:A:164:MET:HE3	1:A:168:LEU:HD11	2.02	0.40
1:A:84:THR:O	1:A:154:LYS:NZ	2.53	0.40
2:B:395:LYS:HZ3	2:B:399:GLU:CG	2.34	0.40
1:A:22:LYS:HG2	1:A:23:GLN:N	2.36	0.40
2:B:21:VAL:CG1	2:B:59:PRO:CG	2.99	0.40
1:A:341:ILE:HG21	1:A:383:TRP:CH2	2.56	0.40
2:B:269:GLN:OE1	2:B:346:PHE:CZ	2.75	0.40
1:A:195:ILE:HG12	1:A:196:GLY:H	1.85	0.40
1:A:171:PHE:CE1	1:A:205:LEU:CA	3.01	0.40
1:A:207:GLN:NE2	1:A:207:GLN:HA	2.36	0.40
2:B:40:GLU:OE2	2:B:40:GLU:HA	2.21	0.40
1:A:393:ILE:HD12	1:A:423:VAL:CG2	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:317:VAL:O	2:B:317:VAL:HG12	2.21	0.40
1:A:216:THR:HB	1:A:217:PRO:HD2	2.03	0.40
2:B:298:GLU:N	2:B:298:GLU:CD	2.73	0.40
1:A:27:THR:CG2	1:A:30:LYS:HG3	2.51	0.40
1:A:26:LEU:HD12	1:A:133:PRO:CG	2.52	0.40
2:B:230:MET:C	2:B:232:TYR:H	2.24	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%)	449 (88%)	45 (9%)	16 (3%)	5	21
2	B	390/440 (89%)	349 (90%)	34 (9%)	7 (2%)	11	37
All	All	900/1000 (90%)	798 (89%)	79 (9%)	23 (3%)	7	26

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	90	VAL
1	A	195	ILE
1	A	222	GLN
1	A	412	PRO
2	B	116	PHE
2	B	428	GLN
1	A	18	GLY
1	A	402	TRP
1	A	418	ASN
2	B	122	GLU
2	B	167	ILE
1	A	137	ASN

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Mol	Chain	Res	Type
1	A	230	MET
1	A	249	LYS
1	A	345	PRO
1	A	356	ARG
1	A	472	THR
2	B	85	GLN
2	B	170	PRO
1	A	91	GLN
1	A	92	LEU
2	B	166	LYS
1	A	170	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	466/499 (93%)	433 (93%)	33 (7%)	18	47
2	B	365/400 (91%)	348 (95%)	17 (5%)	32	68
All	All	831/899 (92%)	781 (94%)	50 (6%)	24	57

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

Mol	Chain	Res	Type
1	A	5	ILE
1	A	6	GLU
1	A	7	THR
1	A	20	LYS
1	A	24	TRP
1	A	39	THR
1	A	74	LEU
1	A	89	GLU
1	A	116	PHE
1	A	135	ILE
1	A	138	GLU
1	A	164	MET

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Mol	Chain	Res	Type
1	A	182	GLN
1	A	195	ILE
1	A	205	LEU
1	A	208	HIS
1	A	215	THR
1	A	218	ASP
1	A	265	ASN
1	A	287	LYS
1	A	301	LEU
1	A	303	LEU
1	A	336	GLN
1	A	340	GLN
1	A	345	PRO
1	A	356	ARG
1	A	428	GLN
1	A	443	ASP
1	A	476	LYS
1	A	484	LEU
1	A	487	GLN
1	A	514	GLU
1	A	517	LEU
2	B	10	VAL
2	B	55	PRO
2	B	109	LEU
2	B	122	GLU
2	B	201	LYS
2	B	205	LEU
2	B	210	LEU
2	B	212	TRP
2	B	232	TYR
2	B	233	GLU
2	B	250	ASP
2	B	295	LEU
2	B	298	GLU
2	B	303	LEU
2	B	413	GLU
2	B	414	TRP
2	B	429	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:



Mol	Chain	Res	Type
1	A	91	GLN
1	A	174	GLN
1	A	207	GLN
1	A	208	HIS
1	A	222	GLN
1	A	242	GLN
1	A	265	ASN
1	A	278	GLN
1	A	315	HIS
1	A	336	GLN
1	A	348	ASN
1	A	475	GLN
1	A	480	GLN
1	A	487	GLN
1	A	500	GLN
1	A	507	GLN
1	A	520	GLN
2	B	57	ASN
2	B	137	ASN
2	B	175	ASN
2	B	207	GLN
2	B	235	HIS
2	B	278	GLN
2	B	336	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	0.69	0	3,8,10	5.06	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	8.55	119.66	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	1.09	0	6,6,6	0.27	0
3	PO4	A	1301	-	4,4,4	1.20	0	6,6,6	0.27	0
3	PO4	A	1302	-	4,4,4	1.06	0	6,6,6	0.27	0
4	H18	A	999	-	21,25,25	2.86	12 (57%)	25,35,35	2.98	8 (32%)

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	H18	A	999	-	-	0/11/19/19	0/3/3/3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	999	H18	C8-CL	-2.56	1.68	1.74
4	A	999	H18	CB-CA	2.10	1.55	1.52
4	A	999	H18	CE-CF	2.21	1.59	1.53
4	A	999	H18	O2-C6	2.23	1.30	1.24
4	A	999	H18	C5-C4	2.55	1.44	1.41
4	A	999	H18	C9-C8	2.56	1.43	1.38
4	A	999	H18	C10-C9	2.96	1.42	1.36
4	A	999	H18	C7-C8	2.99	1.42	1.36
4	A	999	H18	C3-C2	3.77	1.48	1.42
4	A	999	H18	C2-N1	4.43	1.42	1.35
4	A	999	H18	CF-CA	5.75	1.61	1.52
4	A	999	H18	C6-N1	6.63	1.45	1.33

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	999	H18	C3-C2-N1	-3.71	120.06	123.45
4	A	999	H18	C12-C11-C5	-2.82	107.85	112.84
4	A	999	H18	CF-CA-CB	2.28	113.76	111.59
4	A	999	H18	CD-CE-CF	2.61	116.90	111.44
4	A	999	H18	OS-S4-C4	2.69	110.34	106.83
4	A	999	H18	CE-CF-CA	3.36	117.26	110.49
4	A	999	H18	C4-S4-CA	7.77	106.82	97.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	999	H18	C6-N1-C2	9.71	122.78	116.23

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1301	PO4	1	0
4	A	999	H18	5	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	516/560 (92%)	0.26	39 (7%) 17 11	28, 65, 110, 139	0
2	B	400/440 (90%)	0.17	36 (9%) 12 7	28, 60, 117, 148	0
All	All	916/1000 (91%)	0.22	75 (8%) 14 9	28, 64, 113, 148	0

All (75) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	334	GLN	8.1
2	B	214	LEU	6.3
1	A	138	GLU	5.2
2	B	421	PRO	5.2
1	A	116	PHE	5.0
1	A	469	LEU	4.9
1	A	139	THR	4.8
2	B	312	GLU	4.5
1	A	251	SER	4.4
2	B	213	GLY	4.2
2	B	88	TRP	4.0
2	B	197	GLN	3.9
1	A	140	PRO	3.8
1	A	396	GLU	3.8
1	A	472	THR	3.7
2	B	419	THR	3.7
1	A	402	TRP	3.5
1	A	404	GLU	3.5
2	B	96	HIS	3.4
2	B	64	LYS	3.3
1	A	228	LEU	3.3
2	B	212	TRP	3.3
1	A	313	PRO	3.3
2	B	318	TYR	3.3

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Mol	Chain	Res	Type	RSRZ
2	B	426	TRP	3.2
2	B	240	THR	3.2
2	B	204	GLU	3.2
2	B	117	SER	3.2
2	B	362	THR	3.1
1	A	15	GLY	3.1
1	A	20	LYS	3.1
2	B	284	ARG	3.1
2	B	165	THR	3.1
2	B	294	PRO	3.1
2	B	95	PRO	3.1
1	A	82	LYS	3.0
1	A	144	TYR	3.0
1	A	193	LEU	2.9
1	A	27	THR	2.9
1	A	14	PRO	2.9
2	B	420	PRO	2.9
1	A	22	LYS	2.9
2	B	15	GLY	2.8
2	B	191	SER	2.7
1	A	43	LYS	2.6
2	B	425	LEU	2.6
1	A	221	HIS	2.6
2	B	211	ARG	2.5
2	B	277	ARG	2.4
1	A	244	ILE	2.4
2	B	97	PRO	2.4
1	A	287	LYS	2.4
1	A	322	SER	2.4
2	B	104	LYS	2.4
1	A	56	TYR	2.3
1	A	92	LEU	2.3
1	A	346	PHE	2.3
1	A	311	LYS	2.3
1	A	409	THR	2.3
1	A	312	GLU	2.2
1	A	471	ASP	2.2
1	A	344	GLU	2.2
1	A	212	TRP	2.2
2	B	196	GLY	2.2
1	A	210	LEU	2.1
2	B	238	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	516	GLU	2.1
2	B	209	LEU	2.1
1	A	29	GLU	2.0
2	B	313	PRO	2.0
2	B	199	ARG	2.0
1	A	70	LYS	2.0
1	A	113	ASP	2.0
2	B	422	LEU	2.0
2	B	322	SER	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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	0.94	0.17	-	51,55,65,74	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(Å <sup>2</sup> )	Q<0.9
4	H18	A	999	23/23	0.86	0.26	2.50	45,66,78,88	0
3	PO4	A	1301	5/5	0.87	0.23	0.78	123,124,129,131	0
3	PO4	A	1302	5/5	0.88	0.26	-0.28	150,150,150,150	0
3	PO4	A	1300	5/5	0.61	0.20	-0.39	137,140,144,146	0

## 6.5 Other polymers

There are no such residues in this entry.