



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 09:13 AM GMT

PDB ID : 3HNE
Title : Crystal structure of human ribonucleotide reductase 1 bound to the effectors
TTP and ATP
Authors : Fairman, J.W.; Wijerathna, S.R.; Xu, H.; Dealwis, C.G.
Deposited on : 2009-05-31
Resolution : 3.11 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

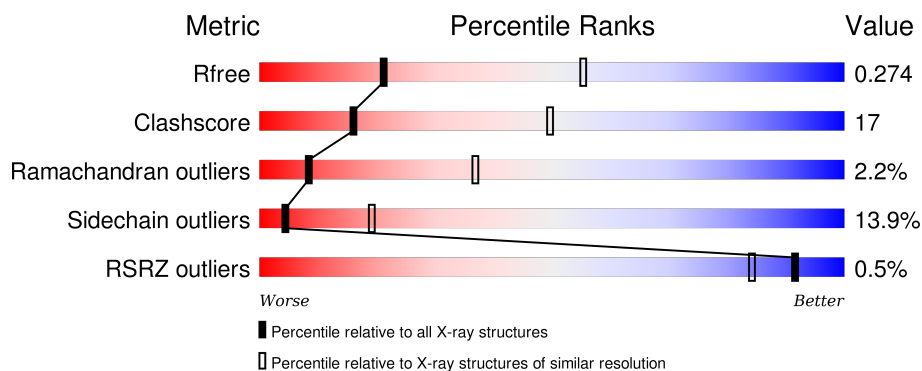
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.11 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	1112 (3.16-3.08)
Clashscore	102246	1218 (3.16-3.08)
Ramachandran outliers	100387	1175 (3.16-3.08)
Sidechain outliers	100360	1175 (3.16-3.08)
RSRZ outliers	91569	1114 (3.16-3.08)

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	792	 61% 24% 5% • 10%
1	B	792	 51% 33% 8% 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
4	SO4	B	813	-	-	-	X

2 Entry composition [i](#)

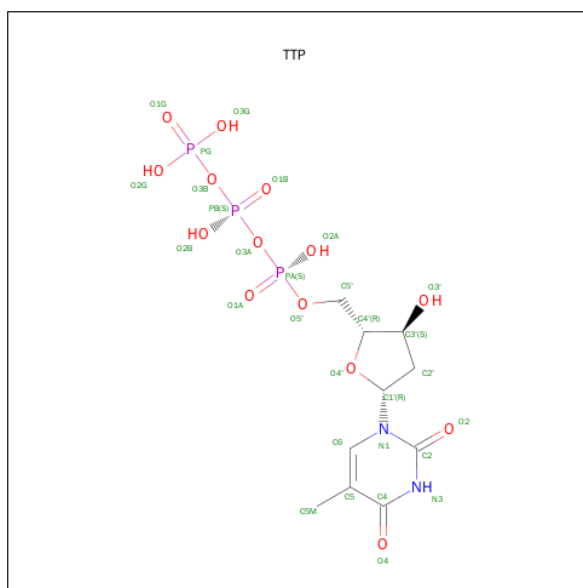
There are 6 unique types of molecules in this entry. The entry contains 11380 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Ribonucleoside-diphosphate reductase large subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	715	Total	C	N	O	S	6	1	0
			5568	3557	927	1051	33			
1	B	724	Total	C	N	O	S	0	0	0
			5644	3593	955	1062	34			

- Molecule 2 is THYMIDINE-5'-TRIPHOSPHATE (three-letter code: TTP) (formula: $C_{10}H_{17}N_2O_{14}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			29	10	2	14	3		
2	B	1	Total	C	N	O	P	0	0
			29	10	2	14	3		

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	3	Total Mg 3 3	0	0
3	A	1	Total Mg 1 1	0	0

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total O S 5 4 1	0	0
4	A	1	Total O S 5 4 1	0	0
4	A	1	Total O S 5 4 1	0	0
4	B	1	Total O S 5 4 1	0	0
4	B	1	Total O S 5 4 1	0	0
4	B	1	Total O S 5 4 1	0	0

- Molecule 5 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	B	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

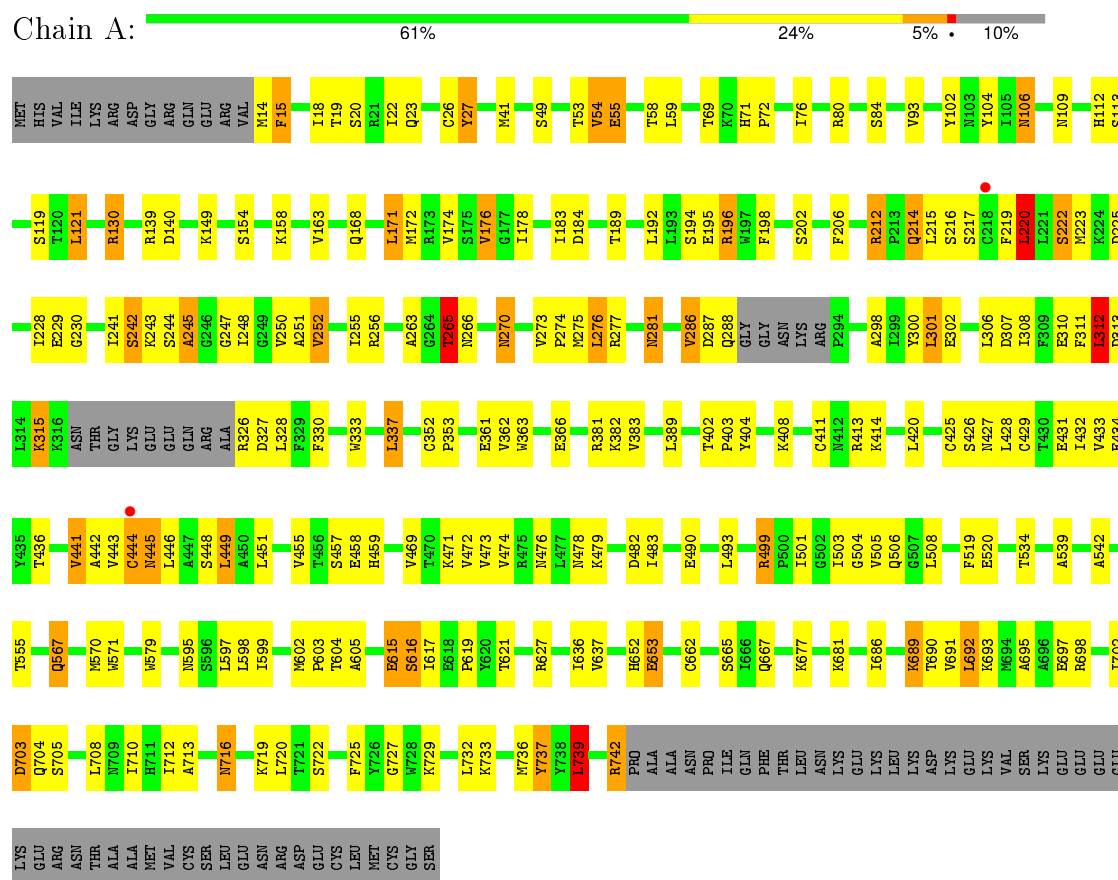
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	27	Total	O	0	0
			27	27		
6	B	18	Total	O	0	0
			18	18		

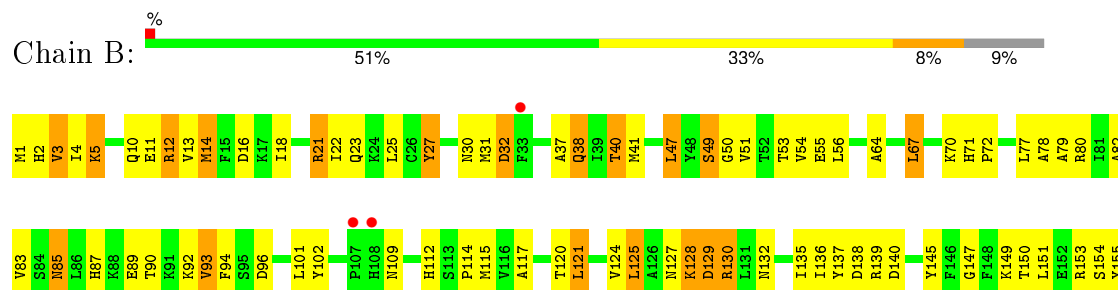
3 Residue-property plots

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: Ribonucleoside-diphosphate reductase large subunit



- Molecule 1: Ribonucleoside-diphosphate reductase large subunit



ASP	E885	I503	K315	V250	
LVS	L686	G504	K316	A251	I159
GLU	S687	V505	K317	V252	
LVS	Q688	Q506	THR	S253	K162
VAL	K689	G507	GLY	C254	
SER	T690	L508	LVS	I255	R166
	V691		GLU	R256	
GLU	L692	F512	GLU	A257	H169
GLU	L611	M515	GLN	T258	M170
	A695	R516	R324	G259	L171
GLU	A696	B517	A325	S260	M172
LVS	E697	P518	R326	I261	R173
GLU	R698	P518	D327	I262	V174
ARG	G699	E523	F330	A263	S175
ASN	A700	E523	F330	G264	V176
THR	F701	E618	D439	T265	
THR	I702	P619	E441	T266	I187
ALA	D703	E620	K333	N266	E188
ALA					
MET	Q704	T621	L337	N270	
VAL	S705	K528	V443	C271	E195
CYS	Q706	S622	C444	L272	R196
SER	S707	R623	K445	V273	
LEU	L708	E625	L446	P274	T199
LEU		E625	A447	P274	
GLU	T826	S448	C352	V275	
ASN	Y717	Y537	P353	L276	S202
ARG	G718	A538	K354	R277	P203
ARG	K719	A539	L359	N281	F206
GLU		LEU	L454	T282	N207
CYS	M723	SER	S457	A283	
LEU	H724	GLY		R284	T210
		GLU	Y461	V286	N211
CYS	G727	F634	E365	D287	R212
GLY	Q635	Q635	F367	Q288	P213
SER	Q730	L645	E368	G289	Q214
				L215	
	T734	G551	Y374	GLY	L216
G735	M651	P552	K471	ASN	S216
T736	H652	Y553	R379	LVS	C217
T737	E653	E554	V474	ARG	R219
Y738	E654	T555	R475	F220	L220
L739	M655		V383	PRO	L221
R740	K656	P560	M476	G295	S222
T741	M657	V561	L477	A296	M223
R742	Q658			F297	
PRO	H659	L566	D482	A298	D226
ALA	I660	Q567	I483	L389	
ALA	A661	Y568	M484	I393	
ASN		D569	Y485	I394	E229
PRO	G664	M570		E392	
ILE			E490	S396	T234
GLN	P673	V673	A491	Q397	
THR	D674	T574	C492	L306	Q237
THR	H675	P575	L493	P403	I241
LEU	L676	T576	R497	V494	
ASN	C677		M405	F405	S244
LVS	Q678	K587	H498	L406	A245
GLU	L679		R499	Y407	
LVS		R594	P500	K408	L312
			I501	D409	I248
LEU	V683	L508	E503	S410	T249
LVS			V503	I249	

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	69.15Å 114.37Å 222.47Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.07 – 3.11 44.07 – 3.11	Depositor EDS
% Data completeness (in resolution range)	88.5 (44.07-3.11) 88.5 (44.07-3.11)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.04 (at 3.12Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.185 , 0.275 0.188 , 0.274	Depositor DCC
R_{free} test set	1440 reflections (5.29%)	DCC
Wilson B-factor (Å ²)	69.4	Xtriage
Anisotropy	0.183	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 45.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 28684 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	11380	wwPDB-VP
Average B, all atoms (Å ²)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.13% 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: MG, TTP, SO4, ATP

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	0.74	3/5696 (0.1%)	0.78	4/7749 (0.1%)
1	B	0.71	2/5767 (0.0%)	0.80	1/7840 (0.0%)
All	All	0.72	5/11463 (0.0%)	0.79	5/15589 (0.0%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	615	GLU	CB-CG	6.68	1.64	1.52
1	B	218	CYS	CB-SG	-6.52	1.71	1.82
1	A	662	CYS	CB-SG	-6.20	1.71	1.82
1	A	615	GLU	CG-CD	5.86	1.60	1.51
1	B	365	GLU	CB-CG	5.49	1.62	1.52

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	449	LEU	CA-CB-CG	7.33	132.16	115.30
1	A	312	LEU	CA-CB-CG	6.74	130.81	115.30
1	A	220	LEU	CA-CB-CG	5.58	128.14	115.30
1	A	739	LEU	CA-CB-CG	5.36	127.62	115.30
1	B	221	LEU	CA-CB-CG	5.14	127.13	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	5568	0	5368	166	0
1	B	5644	0	5448	208	0
2	A	29	0	13	1	0
2	B	29	0	13	4	0
3	A	1	0	0	0	0
3	B	3	0	0	0	0
4	A	15	0	0	2	0
4	B	15	0	0	1	0
5	B	31	0	12	3	0
6	A	27	0	0	3	0
6	B	18	0	0	3	0
All	All	11380	0	10854	374	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 17.

All (374) 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:445:ASN:C	1:A:446:LEU:HD23	1.34	1.44
1:A:445:ASN:O	1:A:446:LEU:HD23	1.50	1.11
1:A:130:ARG:HG2	1:A:130:ARG:HH11	1.18	1.01
1:A:443:VAL:HG12	1:A:444:CYS:H	1.23	0.99
1:A:445:ASN:C	1:A:446:LEU:CD2	2.30	0.98
1:A:567:GLN:HA	1:A:567:GLN:HE21	1.27	0.95
1:B:256:ARG:HD3	2:B:805:TTP:H4'	1.49	0.95
1:B:506:GLN:HA	1:B:616:SER:HA	1.46	0.94
1:A:446:LEU:N	1:A:446:LEU:HD23	1.67	0.94
1:A:443:VAL:HG12	1:A:444:CYS:N	1.80	0.94
1:B:256:ARG:CD	2:B:805:TTP:H4'	1.97	0.94
1:B:568:TYR:HB2	1:B:573:VAL:HG12	1.54	0.87
1:A:534:THR:HG23	1:A:579:TRP:CZ2	2.13	0.84
5:B:807:ATP:O1B	5:B:807:ATP:H5'2	1.80	0.82
1:A:130:ARG:HG2	1:A:130:ARG:NH1	1.93	0.82
1:A:273:VAL:HG23	1:A:274:PRO:HD3	1.63	0.81
1:A:616:SER:OG	1:A:617:ILE:N	2.14	0.80
1:B:619:PRO:HG2	1:B:683:VAL:HG23	1.63	0.80
1:A:742:ARG:HA	1:A:742:ARG:NE	1.95	0.80
1:A:742:ARG:HA	1:A:742:ARG:HE	1.47	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:277:ARG:NH2	1:B:277:ARG:HH22	1.79	0.80
1:B:82:ALA:HA	1:B:85:ASN:OD1	1.81	0.80
1:B:337:LEU:HG	1:B:368:GLU:HG2	1.63	0.79
1:A:445:ASN:O	1:A:446:LEU:CD2	2.30	0.79
1:B:30:ASN:OD1	1:B:32:ASP:HB2	1.83	0.78
1:A:443:VAL:CG1	1:A:444:CYS:H	1.96	0.78
1:B:695:ALA:HB1	1:B:708:LEU:HD11	1.64	0.78
1:A:534:THR:HG23	1:A:579:TRP:HZ2	1.48	0.78
1:B:270:ASN:HB3	1:B:274:PRO:HG2	1.65	0.77
1:A:567:GLN:HA	1:A:567:GLN:NE2	2.00	0.77
1:A:736:MET:SD	1:A:739:LEU:HB2	2.25	0.77
1:B:482:ASP:OD2	1:B:499:ARG:NH2	2.17	0.76
1:A:414:LYS:HG2	1:A:570:MET:HB3	1.66	0.76
1:B:416:ASN:OD1	1:B:561:VAL:HG12	1.85	0.75
1:A:273:VAL:CG2	1:A:274:PRO:HD3	2.18	0.74
1:B:172:MET:O	1:B:176:VAL:HG23	1.89	0.73
1:A:310:GLU:H	1:A:310:GLU:CD	1.90	0.73
1:A:597:LEU:HA	1:A:703:ASP:OD2	1.89	0.72
1:B:482:ASP:CG	1:B:499:ARG:HH22	1.93	0.72
1:A:140:ASP:OD2	1:A:168:GLN:HG2	1.90	0.72
1:B:147:GLY:O	1:B:150:THR:HB	1.90	0.71
1:B:533:GLU:OE2	1:B:576:THR:HG23	1.90	0.71
1:A:245:ALA:HB2	1:A:288:GLN:O	1.90	0.71
1:A:306:LEU:HD13	1:A:381:ARG:HB3	1.73	0.70
1:B:71:HIS:CG	1:B:72:PRO:HD2	2.27	0.70
1:B:71:HIS:CD2	1:B:72:PRO:HD2	2.27	0.70
1:B:420:LEU:HD22	1:B:498:HIS:HE1	1.55	0.69
1:A:474:VAL:HG22	1:A:503:ILE:HD11	1.74	0.69
1:A:14:MET:HE3	1:A:15:PHE:HB3	1.73	0.69
1:B:261:TYR:CE1	1:B:263:ALA:HA	2.28	0.69
1:A:302:GLU:HG2	1:A:333:TRP:HB3	1.74	0.68
1:B:260:SER:OG	1:B:352:CYS:SG	2.50	0.68
1:A:652[B]:HIS:CD2	1:A:653:GLU:H	2.11	0.68
1:A:599:ILE:HG22	1:A:702:ILE:HG23	1.75	0.68
1:B:248:ILE:CD1	1:B:297:PHE:HE2	2.07	0.68
1:A:478:ASN:ND2	1:A:595:ASN:OD1	2.27	0.68
1:B:362:VAL:CG2	1:B:366:GLU:HB3	2.24	0.67
1:B:397:GLN:HG3	1:B:403:PRO:HD2	1.76	0.67
1:A:265:THR:O	1:A:266:ASN:HB2	1.95	0.67
1:A:270:ASN:HB2	1:A:274:PRO:HG2	1.75	0.67
1:B:284:ARG:NH2	1:B:324:ARG:HB3	2.09	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:415:SER:O	1:B:418:GLN:HB2	1.95	0.67
1:B:170:MET:O	1:B:174:VAL:HG23	1.95	0.67
1:B:386:ALA:HB3	6:B:933:HOH:O	1.94	0.66
1:B:475:ARG:HG2	1:B:546:LEU:HD11	1.78	0.66
1:B:374:TYR:HE2	1:B:379:ARG:NH2	1.93	0.66
1:B:223:MET:HG2	1:B:255:ILE:HD11	1.77	0.65
1:B:300:TYR:HE2	1:B:406:LEU:HD13	1.62	0.65
1:A:223:MET:HG2	1:A:255:ILE:HD11	1.79	0.65
1:A:26:CYS:O	1:A:27:TYR:C	2.35	0.64
1:A:298:ALA:HB2	1:A:428:LEU:HA	1.80	0.63
1:B:533:GLU:HG2	1:B:701:PHE:CZ	2.34	0.63
1:A:742:ARG:HE	1:A:742:ARG:CA	2.12	0.63
1:B:568:TYR:HB2	1:B:573:VAL:CG1	2.29	0.62
1:A:652[B]:HIS:CG	1:A:653:GLU:H	2.17	0.62
1:A:71:HIS:CE1	1:A:72:PRO:HD2	2.34	0.62
1:A:241:ILE:CG2	1:A:248:ILE:HD11	2.30	0.62
1:A:420:LEU:HD21	1:A:555:THR:HB	1.82	0.62
1:B:121:LEU:HD22	1:B:125:LEU:HD12	1.82	0.62
1:B:93:VAL:HG13	1:B:96:ASP:HB2	1.81	0.61
1:B:315:LYS:HD2	1:B:326:ARG:HG2	1.82	0.61
1:B:689:LYS:HB2	4:B:810:SO4:O3	2.01	0.61
1:A:429:CYS:HB2	1:A:431:GLU:OE2	2.01	0.60
1:B:302:GLU:HG2	1:B:333:TRP:HB3	1.84	0.60
1:A:71:HIS:ND1	1:A:72:PRO:HD2	2.17	0.60
1:B:493:LEU:HD11	1:B:497:ARG:NH1	2.17	0.60
1:B:308:ILE:O	1:B:311:PHE:HB3	2.02	0.60
1:A:446:LEU:HB3	1:A:602:MET:HE2	1.83	0.60
1:B:94:PHE:CE1	1:B:172:MET:HB3	2.37	0.59
1:B:206:PHE:HB3	1:B:207:ASN:HD22	1.67	0.59
1:B:394:ILE:HD12	1:B:395:GLU:N	2.17	0.59
1:B:89:GLU:O	1:B:90:THR:HB	2.02	0.59
1:A:474:VAL:HG21	1:A:539:ALA:HA	1.84	0.59
1:A:270:ASN:H	1:A:270:ASN:ND2	2.00	0.59
1:B:37:ALA:O	1:B:41:MET:HG2	2.03	0.59
1:A:251:ALA:HB2	1:A:425:CYS:HB3	1.85	0.59
1:B:248:ILE:HD13	1:B:297:PHE:CE2	2.39	0.58
1:A:225:ASP:HB3	1:A:230:GLY:HA3	1.85	0.58
1:A:219:PHE:N	1:A:247:GLY:O	2.35	0.58
1:A:352:CYS:HB3	1:A:381:ARG:NH2	2.18	0.58
1:A:501:ILE:HG13	1:A:598:LEU:HA	1.84	0.57
1:A:214:GLN:HG3	1:A:244:SER:CB	2.34	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:206:PHE:CB	1:B:207:ASN:HD22	2.17	0.57
5:B:807:ATP:C5'	5:B:807:ATP:O1B	2.52	0.57
1:B:408:LYS:HD3	6:B:924:HOH:O	2.04	0.57
1:A:14:MET:CE	1:A:15:PHE:HB3	2.33	0.57
1:A:698:ARG:O	1:A:702:ILE:HG13	2.04	0.57
1:B:117:ALA:H	1:B:210:THR:HA	1.69	0.57
1:B:248:ILE:HD13	1:B:297:PHE:HE2	1.70	0.57
1:A:315:LYS:HZ1	1:A:326:ARG:HA	1.70	0.57
1:B:553:TYR:HB3	1:B:594:ARG:O	2.04	0.57
1:B:218:CYS:O	1:B:443:VAL:HA	2.05	0.57
1:A:426:SER:OG	1:A:427:ASN:N	2.38	0.56
1:B:346:GLN:HG3	1:B:347:ASP:H	1.69	0.56
1:A:433:VAL:H	1:A:704:GLN:HB3	1.71	0.56
1:A:18:ILE:O	1:A:22:ILE:HG12	2.06	0.56
1:A:76:ILE:O	1:A:80:ARG:HG3	2.06	0.56
1:A:222:SER:OG	1:A:436:THR:OG1	2.22	0.56
1:A:441:VAL:HG13	1:A:490:GLU:HB3	1.86	0.56
1:B:83:VAL:HG11	1:B:140:ASP:HB3	1.86	0.55
1:B:18:ILE:HB	1:B:40:THR:HG23	1.87	0.55
1:B:673:PRO:HB2	1:B:675:ASP:OD1	2.06	0.55
1:A:219:PHE:CE2	1:A:443:VAL:HG22	2.42	0.55
1:B:443:VAL:CG2	1:B:491:ALA:HB1	2.37	0.55
1:B:166:ARG:HD2	1:B:169:HIS:CE1	2.42	0.55
1:B:675:ASP:N	1:B:675:ASP:OD1	2.39	0.55
1:B:651:TRP:CD1	1:B:651:TRP:C	2.80	0.55
1:B:625:TYR:HD1	1:B:625:TYR:C	2.11	0.55
1:A:432:ILE:HG22	1:A:434:GLU:HG3	1.89	0.54
1:B:248:ILE:CD1	1:B:297:PHE:CE2	2.90	0.54
1:B:287:ASP:C	1:B:289:GLY:H	2.10	0.54
1:A:471:LYS:HA	1:A:542:ALA:HB2	1.89	0.54
1:B:129:ASP:N	1:B:129:ASP:OD2	2.37	0.54
1:A:308:ILE:O	1:A:312:LEU:HD22	2.07	0.54
1:A:627:ARG:HG2	1:A:636:ILE:HD12	1.89	0.54
1:A:652[B]:HIS:CD2	1:A:653:GLU:N	2.76	0.54
1:A:228:ILE:O	1:A:229:GLU:C	2.45	0.54
1:B:87:HIS:NE2	1:B:140:ASP:OD1	2.30	0.54
1:B:405:MET:HG3	1:B:724:HIS:CE1	2.43	0.54
1:B:448:SER:HA	1:B:504:GLY:O	2.07	0.54
1:B:443:VAL:HG12	1:B:444:CYS:N	2.22	0.54
1:B:256:ARG:HG3	1:B:354:ASN:HB2	1.90	0.53
1:A:172:MET:O	1:A:176:VAL:HG22	2.07	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:416:ASN:HA	1:B:560:PRO:HG2	1.91	0.53
1:A:695:ALA:HA	1:A:698:ARG:NH1	2.23	0.53
1:B:248:ILE:HD12	1:B:297:PHE:HE2	1.73	0.53
1:B:287:ASP:O	1:B:289:GLY:N	2.38	0.53
1:B:79:ALA:HB2	1:B:145:TYR:N	2.23	0.53
1:B:284:ARG:CZ	1:B:324:ARG:HB3	2.38	0.53
1:A:315:LYS:NZ	1:A:326:ARG:HA	2.23	0.53
1:A:174:VAL:HG12	1:A:178:ILE:HD12	1.91	0.53
1:B:195:GLU:C	1:B:196:ARG:HG3	2.29	0.53
1:B:102:TYR:CG	1:B:121:LEU:HD12	2.44	0.53
1:A:315:LYS:NZ	1:A:328:LEU:O	2.42	0.52
1:B:727:GLY:O	1:B:730:GLN:HB2	2.08	0.52
1:B:624:ILE:HG22	1:B:664:GLY:HA2	1.91	0.52
1:A:479:LYS:HA	6:A:910:HOH:O	2.10	0.52
1:B:326:ARG:O	1:B:327:ASP:HB2	2.08	0.52
1:A:212:ARG:O	1:A:214:GLN:N	2.37	0.52
1:B:687:SER:HB3	1:B:690:THR:OG1	2.09	0.52
1:B:696:ALA:O	1:B:699:GLY:N	2.42	0.52
1:B:64:ALA:HB3	1:B:78:ALA:HB2	1.90	0.52
1:B:420:LEU:HD22	1:B:498:HIS:CE1	2.40	0.52
1:B:362:VAL:HG23	1:B:366:GLU:OE2	2.10	0.52
1:A:27:TYR:O	1:A:80:ARG:NH2	2.42	0.51
1:B:346:GLN:CG	1:B:347:ASP:H	2.23	0.51
1:B:394:ILE:HD11	1:B:717:TYR:CE1	2.45	0.51
1:B:394:ILE:C	1:B:394:ILE:HD12	2.30	0.51
1:A:198:PHE:CE2	1:A:473:VAL:HG22	2.45	0.51
1:A:382:LYS:HG2	1:A:383:VAL:N	2.26	0.51
1:B:601:PRO:HG2	1:B:702:ILE:HD13	1.91	0.51
1:B:3:VAL:HG23	1:B:11:GLU:O	2.10	0.51
1:A:189:THR:CG2	1:A:476:ASN:HD21	2.23	0.51
1:A:139:ARG:HD3	1:A:194:SER:HB2	1.91	0.51
1:B:625:TYR:CD1	1:B:625:TYR:C	2.84	0.51
1:A:310:GLU:HA	1:A:313:ASP:HB2	1.93	0.51
1:B:602:MET:HB2	1:B:603:PRO:HD2	1.93	0.51
1:A:652[B]:HIS:CG	1:A:653:GLU:N	2.77	0.50
1:B:212:ARG:HG2	1:B:485:TYR:CZ	2.46	0.50
1:B:101:LEU:O	1:B:115:MET:HB2	2.11	0.50
1:A:195:GLU:O	1:A:196:ARG:HB2	2.11	0.50
1:B:454:TYR:HB2	1:B:461:TYR:CZ	2.46	0.50
1:A:402:THR:HB	1:A:403:PRO:HA	1.92	0.50
1:A:520:GLU:HB2	1:A:690:THR:HG21	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:464:LYS:O	1:B:468:GLU:HG2	2.11	0.50
1:B:1:MET:HE1	1:B:47:LEU:HD12	1.93	0.50
1:B:443:VAL:HG23	1:B:491:ALA:HB1	1.93	0.50
1:A:362:VAL:CG2	1:A:366:GLU:HB2	2.42	0.50
1:B:474:VAL:HG21	1:B:539:ALA:HA	1.93	0.50
1:B:22:ILE:HG23	1:B:77:LEU:HD21	1.94	0.50
1:A:275:MET:CE	1:A:276:LEU:CD1	2.90	0.50
1:B:734:THR:HG22	1:B:736:MET:H	1.76	0.49
1:B:532:PHE:CE2	1:B:698:ARG:HD3	2.47	0.49
1:A:310:GLU:N	1:A:310:GLU:CD	2.61	0.49
1:B:735:GLY:O	1:B:736:MET:HB2	2.11	0.49
1:B:420:LEU:CD2	1:B:498:HIS:HE1	2.23	0.49
1:B:261:TYR:CE2	1:B:266:ASN:O	2.66	0.49
1:B:206:PHE:HB3	1:B:207:ASN:ND2	2.27	0.49
1:B:541:GLU:O	1:B:542:ALA:C	2.49	0.49
1:B:446:LEU:HD13	1:B:602:MET:HG3	1.94	0.49
1:A:26:CYS:O	1:A:27:TYR:O	2.30	0.49
1:B:567:GLN:CD	1:B:703:ASP:HA	2.32	0.49
1:B:374:TYR:CE2	1:B:379:ARG:NH2	2.77	0.49
1:A:242:SER:HB3	1:A:286:VAL:HG22	1.95	0.49
1:B:498:HIS:CE1	1:B:555:THR:HG21	2.48	0.49
1:A:333:TRP:CD1	1:A:408:LYS:HD2	2.48	0.49
1:A:716:ASN:O	1:A:719:LYS:N	2.46	0.49
1:B:695:ALA:CB	1:B:708:LEU:HD11	2.39	0.48
1:A:71:HIS:CG	1:A:72:PRO:CD	2.97	0.48
1:B:441:VAL:O	1:B:491:ALA:HA	2.14	0.48
1:A:482:ASP:OD1	1:A:499:ARG:NH2	2.47	0.48
1:A:102:TYR:CG	1:A:121:LEU:HD12	2.48	0.48
1:B:220:LEU:N	1:B:220:LEU:HD23	2.29	0.48
1:B:94:PHE:HB2	1:B:135:ILE:CD1	2.44	0.48
1:A:219:PHE:HB2	1:A:247:GLY:O	2.14	0.48
1:B:171:LEU:HD12	1:B:171:LEU:HA	1.62	0.48
1:B:277:ARG:O	1:B:281:ASN:HB2	2.14	0.48
1:B:443:VAL:CG1	1:B:444:CYS:N	2.77	0.48
1:A:457:SER:C	1:A:459:HIS:H	2.17	0.48
1:B:4:ILE:O	1:B:53:THR:HG23	2.14	0.48
1:A:220:LEU:HG	1:A:442:ALA:HB3	1.95	0.48
1:B:300:TYR:CE2	1:B:406:LEU:HD13	2.46	0.47
1:A:431:GLU:HG2	1:A:432:ILE:CD1	2.44	0.47
1:A:692:LEU:CD1	1:A:710:ILE:HD11	2.44	0.47
1:A:432:ILE:CG2	1:A:434:GLU:HG3	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:652:HIS:CG	1:B:653:GLU:H	2.32	0.47
1:A:202:SER:OG	4:A:812:SO4:O4	2.29	0.47
1:B:448:SER:HB2	1:B:506:GLN:HG2	1.97	0.47
1:B:544:CYS:SG	1:B:587:LYS:HG2	2.54	0.47
1:A:330:PHE:N	1:A:330:PHE:CD2	2.83	0.47
1:B:237:GLN:O	1:B:241:ILE:HG13	2.14	0.47
1:B:518:PRO:HB3	1:B:678:GLN:O	2.15	0.47
1:A:183:ILE:O	1:A:184:ASP:C	2.52	0.47
1:A:411:CYS:HA	1:A:733:LYS:HG2	1.95	0.47
1:B:27:TYR:HE1	1:B:80:ARG:NH1	2.13	0.47
1:B:273:VAL:HG21	1:B:310:GLU:HB3	1.97	0.47
1:A:443:VAL:CG1	1:A:444:CYS:N	2.52	0.47
1:A:427:ASN:HB2	6:A:903:HOH:O	2.14	0.47
1:B:130:ARG:NH1	1:B:187:ILE:HD13	2.29	0.47
1:B:5:LYS:HE2	1:B:11:GLU:CD	2.34	0.47
1:A:275:MET:HE1	1:A:276:LEU:CD1	2.44	0.47
1:B:257:ALA:HB1	1:B:306:LEU:HD23	1.97	0.46
1:B:137:TYR:HE2	1:B:169:HIS:NE2	2.13	0.46
1:B:610:ILE:HG22	1:B:611:LEU:HD23	1.96	0.46
1:A:202:SER:HB3	1:A:206:PHE:CE1	2.51	0.46
1:A:198:PHE:CD2	1:A:473:VAL:HG22	2.51	0.46
1:B:695:ALA:O	1:B:706:GLN:NE2	2.49	0.46
1:B:542:ALA:O	1:B:546:LEU:HD12	2.16	0.46
1:B:94:PHE:HB2	1:B:135:ILE:HD13	1.98	0.45
1:B:261:TYR:HE2	1:B:266:ASN:O	1.98	0.45
1:A:192:LEU:HD23	1:A:469:VAL:HG13	1.96	0.45
1:B:49:SER:O	1:B:51:VAL:N	2.49	0.45
1:B:420:LEU:CD2	1:B:498:HIS:CE1	3.00	0.45
1:B:79:ALA:O	1:B:83:VAL:HG23	2.16	0.45
1:B:508:LEU:HD13	1:B:512:PHE:CE2	2.51	0.45
1:B:199:THR:HG21	1:B:607:THR:HB	1.97	0.45
1:B:315:LYS:NZ	1:B:326:ARG:HB3	2.32	0.45
1:B:408:LYS:HE3	6:B:926:HOH:O	2.15	0.45
1:B:220:LEU:HD22	1:B:427:ASN:HB3	1.97	0.45
1:A:667:GLN:O	1:A:677:LYS:HE2	2.17	0.45
1:B:21:ARG:O	1:B:21:ARG:HD2	2.16	0.45
1:B:218:CYS:SG	1:B:432:ILE:HG13	2.56	0.45
1:A:681:LYS:HB2	1:A:686:ILE:HD11	1.99	0.45
1:A:158:LYS:HD3	1:A:163:VAL:HG23	1.98	0.45
1:A:71:HIS:ND1	1:A:72:PRO:CD	2.80	0.45
1:A:26:CYS:C	1:A:27:TYR:O	2.48	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:622:SER:OG	1:B:664:GLY:HA3	2.15	0.45
1:B:250:VAL:N	1:B:298:ALA:O	2.47	0.45
1:B:202:SER:O	1:B:203:PRO:C	2.56	0.44
1:A:281:ASN:HD22	1:A:281:ASN:HA	1.52	0.44
1:A:665:SER:OG	1:A:667:GLN:HG2	2.17	0.44
1:B:22:ILE:CG2	1:B:77:LEU:HD21	2.48	0.44
1:B:652:HIS:CD2	1:B:653:GLU:H	2.36	0.44
1:B:493:LEU:CD1	1:B:497:ARG:NH1	2.80	0.44
1:A:519:PHE:CE2	1:A:619:PRO:HG3	2.53	0.44
1:A:215:LEU:HD11	1:A:483:ILE:HD11	1.99	0.44
1:A:602:MET:N	1:A:602:MET:SD	2.89	0.44
1:B:207:ASN:O	1:B:210:THR:OG1	2.28	0.44
1:A:275:MET:CE	1:A:276:LEU:HD12	2.48	0.44
1:B:451:LEU:CD1	1:B:508:LEU:HD23	2.48	0.44
1:A:363:TRP:CH2	1:A:413:ARG:HA	2.53	0.44
1:B:2:HIS:ND1	1:B:10:GLN:HG2	2.33	0.44
1:B:312:LEU:HD21	1:B:393:ILE:HG12	1.99	0.44
1:B:501:ILE:HG13	1:B:598:LEU:HA	1.99	0.44
1:B:214:GLN:HG3	1:B:244:SER:HB3	2.00	0.44
1:A:742:ARG:CA	1:A:742:ARG:NE	2.71	0.43
1:B:451:LEU:HD13	1:B:508:LEU:HD23	2.00	0.43
1:B:120:THR:O	1:B:124:VAL:HG23	2.18	0.43
1:A:404:TYR:CZ	1:A:737:TYR:HE1	2.37	0.43
1:B:708:LEU:O	1:B:737:TYR:HB3	2.18	0.43
1:A:308:ILE:O	1:A:311:PHE:HB3	2.18	0.43
1:B:136:ILE:HB	1:B:139:ARG:HG3	2.00	0.43
1:A:216:SER:HB3	1:A:443:VAL:CG1	2.48	0.43
1:B:226:ASP:OD1	1:B:256:ARG:HD2	2.18	0.43
1:B:346:GLN:HG3	1:B:347:ASP:N	2.33	0.43
1:B:653:GLU:O	1:B:655:MET:N	2.51	0.43
1:A:337:LEU:HD22	1:A:337:LEU:HA	1.74	0.43
1:B:283:ALA:HB2	1:B:297:PHE:CD1	2.54	0.43
1:B:362:VAL:HG23	1:B:366:GLU:HB3	1.98	0.43
1:A:252:VAL:HG12	1:A:300:TYR:O	2.18	0.43
1:B:523:GLU:N	1:B:523:GLU:OE2	2.31	0.42
1:A:216:SER:CB	1:A:443:VAL:CG1	2.96	0.42
1:A:690:THR:O	1:A:691:VAL:C	2.57	0.42
1:A:265:THR:CG2	1:B:288:GLN:HG2	2.50	0.42
1:A:256:ARG:HA	1:A:353:PRO:HD2	2.01	0.42
1:A:263:ALA:HB3	2:A:806:TTP:O1G	2.20	0.42
1:B:256:ARG:HH21	1:B:262:ILE:HA	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:551:GLY:O	1:B:594:ARG:NH1	2.50	0.42
1:B:3:VAL:HG22	1:B:13:VAL:HG22	2.01	0.42
1:B:23:GLN:HE22	1:B:31:MET:HE2	1.85	0.42
1:B:256:ARG:HD2	2:B:805:TTP:H4'	1.91	0.42
1:A:414:LYS:HD2	1:A:571:TRP:NE1	2.35	0.42
1:A:265:THR:HG21	1:B:288:GLN:HG2	2.01	0.42
1:B:611:LEU:HB2	1:B:613:ASN:HD22	1.85	0.42
1:A:20:SER:O	1:A:23:GLN:HB3	2.19	0.42
1:A:54:VAL:HG13	1:A:55:GLU:HG3	2.00	0.42
1:A:106:ASN:HD21	1:A:109:ASN:H	1.67	0.42
1:B:483:ILE:HA	1:B:483:ILE:HD12	1.92	0.42
1:A:307:ASP:C	1:A:310:GLU:OE1	2.57	0.42
1:A:627:ARG:CG	1:A:636:ILE:HD12	2.49	0.42
1:B:112:HIS:CE1	1:B:114:PRO:HG3	2.55	0.42
1:B:515:MET:O	1:B:516:ARG:HB2	2.18	0.42
1:B:83:VAL:CG1	1:B:140:ASP:HB3	2.48	0.42
1:A:241:ILE:HG22	1:A:248:ILE:HD11	2.01	0.42
1:B:441:VAL:HG12	1:B:490:GLU:HB2	2.02	0.42
1:B:414:LYS:HG2	1:B:570:MET:HB2	2.01	0.42
1:A:71:HIS:CG	1:A:72:PRO:HD2	2.55	0.41
1:B:516:ARG:HH21	1:B:679:LEU:CD1	2.33	0.41
1:B:645:LEU:HA	1:B:645:LEU:HD23	1.87	0.41
1:B:308:ILE:HG13	1:B:312:LEU:HD13	2.02	0.41
1:B:219:PHE:CE2	1:B:443:VAL:HG22	2.55	0.41
1:A:106:ASN:ND2	1:A:109:ASN:H	2.18	0.41
1:B:222:SER:HA	1:B:251:ALA:HB3	2.02	0.41
1:B:626:THR:HG22	1:B:635:GLN:HA	2.01	0.41
1:B:445:ASN:ND2	1:B:445:ASN:N	2.68	0.41
1:A:446:LEU:N	1:A:446:LEU:CD2	2.43	0.41
1:B:67:LEU:O	1:B:70:LYS:N	2.52	0.41
5:B:807:ATP:PB	5:B:807:ATP:H5'2	2.60	0.41
1:B:300:TYR:HE2	1:B:406:LEU:CD1	2.30	0.41
1:A:330:PHE:N	1:A:330:PHE:HD2	2.19	0.41
1:B:38:GLN:HA	1:B:38:GLN:NE2	2.35	0.41
1:B:566:LEU:O	1:B:567:GLN:C	2.58	0.41
1:B:528:ASN:O	1:B:529:LYS:C	2.59	0.41
1:B:330:PHE:N	1:B:330:PHE:CD2	2.88	0.41
1:A:451:LEU:HG	1:A:505:VAL:HB	2.02	0.41
1:A:689:LYS:HB2	4:A:809:SO4:O1	2.21	0.41
1:A:171:LEU:HD23	1:A:194:SER:HA	2.03	0.41
1:B:272:LEU:HD23	1:B:272:LEU:HA	1.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:270:ASN:N	1:A:270:ASN:ND2	2.67	0.41
1:B:705:SER:OG	1:B:706:GLN:N	2.54	0.41
1:A:520:GLU:HG2	6:A:914:HOH:O	2.21	0.41
1:A:692:LEU:HD13	1:A:710:ILE:HD11	2.03	0.41
1:B:12:ARG:HH21	1:B:14:MET:CE	2.34	0.41
1:B:253:SER:OG	1:B:301:LEU:HD23	2.21	0.41
1:A:603:PRO:O	1:A:604:THR:C	2.59	0.41
1:B:471:LYS:HA	1:B:542:ALA:HB2	2.02	0.41
1:B:128:LYS:O	1:B:132:ASN:ND2	2.49	0.41
1:A:192:LEU:HD22	1:A:472:VAL:HG11	2.03	0.40
1:A:725:PHE:O	1:A:729:LYS:HB2	2.21	0.40
1:A:104:TYR:HD2	1:A:113:SER:HB2	1.86	0.40
1:B:365:GLU:HG2	1:B:365:GLU:H	1.43	0.40
1:A:448:SER:HB2	1:A:506:GLN:HG2	2.03	0.40
1:B:337:LEU:HD23	1:B:337:LEU:HA	1.95	0.40
1:A:301:LEU:HD12	1:A:311:PHE:CG	2.56	0.40
1:B:151:LEU:HD23	1:B:155:TYR:HB2	2.03	0.40
1:B:533:GLU:HG2	1:B:701:PHE:CE1	2.55	0.40
1:A:695:ALA:CB	1:A:708:LEU:HD11	2.51	0.40
1:A:275:MET:HE2	1:A:276:LEU:CD1	2.51	0.40
1:A:215:LEU:CD1	1:A:483:ILE:HD11	2.51	0.40
1:A:727:GLY:CA	1:A:732:LEU:HD12	2.51	0.40
1:A:243:LYS:NZ	2:B:805:TTP:O1B	2.52	0.40
1:B:93:VAL:HG23	1:B:132:ASN:OD1	2.22	0.40
1:A:448:SER:HA	1:A:504:GLY:O	2.22	0.40
1:B:477:LEU:HA	1:B:477:LEU:HD23	1.86	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	710/792 (90%)	636 (90%)	61 (9%)	13 (2%)	11	43
1	B	716/792 (90%)	616 (86%)	82 (12%)	18 (2%)	7	33
All	All	1426/1584 (90%)	1252 (88%)	143 (10%)	31 (2%)	8	37

All (31) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	327	ASP
1	B	130	ARG
1	B	288	GLN
1	B	316	LYS
1	B	327	ASP
1	B	653	GLU
1	B	654	GLU
1	A	245	ALA
1	A	444	CYS
1	A	458	GLU
1	A	605	ALA
1	A	616	SER
1	A	713	ALA
1	A	737	TYR
1	B	50	GLY
1	B	484	ASN
1	B	736	MET
1	B	128	LYS
1	B	258	THR
1	B	313	ASP
1	B	576	THR
1	B	661	ALA
1	B	737	TYR
1	A	112	HIS
1	A	196	ARG
1	B	537	TYR
1	A	49	SER
1	A	265	THR
1	B	303	PRO
1	B	245	ALA
1	A	212	ARG

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	586/693 (85%)	523 (89%)	63 (11%)	8	31
1	B	593/693 (86%)	492 (83%)	101 (17%)	2	11
All	All	1179/1386 (85%)	1015 (86%)	164 (14%)	4	19

All (164) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	PHE
1	A	19	THR
1	A	27	TYR
1	A	41	MET
1	A	53	THR
1	A	54	VAL
1	A	55	GLU
1	A	58	THR
1	A	59	LEU
1	A	69	THR
1	A	84	SER
1	A	93	VAL
1	A	106	ASN
1	A	119	SER
1	A	121	LEU
1	A	130	ARG
1	A	149	LYS
1	A	154	SER
1	A	171	LEU
1	A	176	VAL
1	A	214	GLN
1	A	217	SER
1	A	220	LEU
1	A	222	SER
1	A	242	SER
1	A	250	VAL
1	A	252	VAL

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Mol	Chain	Res	Type
1	A	265	THR
1	A	270	ASN
1	A	276	LEU
1	A	281	ASN
1	A	286	VAL
1	A	287	ASP
1	A	301	LEU
1	A	312	LEU
1	A	315	LYS
1	A	337	LEU
1	A	361	GLU
1	A	389	LEU
1	A	441	VAL
1	A	445	ASN
1	A	449	LEU
1	A	455	VAL
1	A	493	LEU
1	A	499	ARG
1	A	508	LEU
1	A	567	GLN
1	A	615	GLU
1	A	621	THR
1	A	637	VAL
1	A	653	GLU
1	A	689	LYS
1	A	692	LEU
1	A	693	LYS
1	A	697	GLU
1	A	703	ASP
1	A	705	SER
1	A	712	ILE
1	A	716	ASN
1	A	720	LEU
1	A	722	SER
1	A	739	LEU
1	A	742	ARG
1	B	3	VAL
1	B	5	LYS
1	B	12	ARG
1	B	14	MET
1	B	16	ASP
1	B	21	ARG

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Mol	Chain	Res	Type
1	B	25	LEU
1	B	27	TYR
1	B	32	ASP
1	B	38	GLN
1	B	40	THR
1	B	47	LEU
1	B	49	SER
1	B	54	VAL
1	B	55	GLU
1	B	56	LEU
1	B	67	LEU
1	B	85	ASN
1	B	92	LYS
1	B	93	VAL
1	B	109	ASN
1	B	121	LEU
1	B	125	LEU
1	B	127	ASN
1	B	129	ASP
1	B	138	ASP
1	B	149	LYS
1	B	153	ARG
1	B	154	SER
1	B	159	ILE
1	B	162	LYS
1	B	171	LEU
1	B	175	SER
1	B	188	GLU
1	B	196	ARG
1	B	214	GLN
1	B	216	SER
1	B	218	CYS
1	B	220	LEU
1	B	229	GLU
1	B	234	THR
1	B	237	GLN
1	B	241	ILE
1	B	252	VAL
1	B	256	ARG
1	B	265	THR
1	B	272	LEU
1	B	276	LEU

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Mol	Chain	Res	Type
1	B	277	ARG
1	B	286	VAL
1	B	301	LEU
1	B	313	ASP
1	B	314	LEU
1	B	324	ARG
1	B	326	ARG
1	B	337	LEU
1	B	352	CYS
1	B	359	LEU
1	B	365	GLU
1	B	366	GLU
1	B	383	VAL
1	B	389	LEU
1	B	410	SER
1	B	420	LEU
1	B	426	SER
1	B	439	ASP
1	B	441	VAL
1	B	445	ASN
1	B	457	SER
1	B	503	ILE
1	B	506	GLN
1	B	508	LEU
1	B	525	GLN
1	B	541	GLU
1	B	546	LEU
1	B	570	MET
1	B	573	VAL
1	B	575	PRO
1	B	587	LYS
1	B	602	MET
1	B	615	GLU
1	B	618	GLU
1	B	620	TYR
1	B	625	TYR
1	B	626	THR
1	B	655	MET
1	B	657	ASN
1	B	675	ASP
1	B	678	GLN
1	B	683	VAL

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Mol	Chain	Res	Type
1	B	685	GLU
1	B	690	THR
1	B	692	LEU
1	B	697	GLU
1	B	707	SER
1	B	708	LEU
1	B	719	LYS
1	B	723	MET
1	B	739	LEU
1	B	740	ARG
1	B	742	ARG

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	38	GLN
1	A	106	ASN
1	A	200	HIS
1	A	211	ASN
1	A	270	ASN
1	A	281	ASN
1	A	387	GLN
1	A	388	GLN
1	A	476	ASN
1	A	478	ASN
1	A	567	GLN
1	A	595	ASN
1	A	716	ASN
1	B	23	GLN
1	B	38	GLN
1	B	109	ASN
1	B	207	ASN
1	B	214	GLN
1	B	281	ASN
1	B	445	ASN
1	B	459	HIS
1	B	525	GLN
1	B	652	HIS
1	B	711	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 13 ligands modelled in this entry, 4 are monoatomic - leaving 9 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
2	TTP	A	806	3	21,30,30	0.53	0	31,47,47	2.02	6 (19%)
4	SO4	A	808	-	4,4,4	0.14	0	6,6,6	0.31	0
4	SO4	A	809	-	4,4,4	0.17	0	6,6,6	0.30	0
4	SO4	A	812	-	4,4,4	0.18	0	6,6,6	0.57	0
2	TTP	B	805	3	21,30,30	0.58	0	31,47,47	2.04	4 (12%)
5	ATP	B	807	3	24,33,33	1.39	2 (8%)	31,52,52	2.27	8 (25%)
4	SO4	B	810	-	4,4,4	0.20	0	6,6,6	0.26	0
4	SO4	B	811	-	4,4,4	0.18	0	6,6,6	0.57	0
4	SO4	B	813	-	4,4,4	0.32	0	6,6,6	0.41	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	TTP	A	806	3	-	0/18/34/34	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	SO4	A	808	-	-	0/0/0/0	0/0/0/0
4	SO4	A	809	-	-	0/0/0/0	0/0/0/0
4	SO4	A	812	-	-	0/0/0/0	0/0/0/0
2	TTP	B	805	3	-	0/18/34/34	0/2/2/2
5	ATP	B	807	3	-	0/18/38/38	0/3/3/3
4	SO4	B	810	-	-	0/0/0/0	0/0/0/0
4	SO4	B	811	-	-	0/0/0/0	0/0/0/0
4	SO4	B	813	-	-	0/0/0/0	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	807	ATP	C5-C4	3.24	1.47	1.40
5	B	807	ATP	O4'-C1'	4.95	1.47	1.41

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	805	TTP	C5-C4-N3	-5.62	118.88	125.14
2	A	806	TTP	C5-C4-N3	-5.57	118.94	125.14
5	B	807	ATP	PA-O3A-PB	-5.36	117.67	132.73
5	B	807	ATP	N3-C2-N1	-5.27	124.86	128.89
2	A	806	TTP	PB-O3A-PA	-4.92	118.92	132.73
2	B	805	TTP	PB-O3A-PA	-4.38	120.43	132.73
5	B	807	ATP	C4-C5-N7	-4.18	105.64	109.48
5	B	807	ATP	C2'-C1'-N9	-4.13	107.98	114.29
2	A	806	TTP	PB-O3B-PG	-3.66	120.41	132.67
2	B	805	TTP	PB-O3B-PG	-3.01	122.57	132.67
2	A	806	TTP	O2B-PB-O3A	2.12	114.71	105.09
5	B	807	ATP	O3G-PG-O2G	2.65	117.47	107.38
5	B	807	ATP	O4'-C4'-C5'	2.79	119.31	109.32
2	A	806	TTP	O2B-PB-O3B	2.81	117.83	105.09
5	B	807	ATP	O4'-C1'-N9	3.03	114.45	108.10
5	B	807	ATP	O3G-PG-O1G	3.06	120.45	110.58
2	A	806	TTP	C4-N3-C2	5.87	120.32	115.25
2	B	805	TTP	C4-N3-C2	6.92	121.22	115.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	806	TTP	1	0
4	A	809	SO4	1	0
4	A	812	SO4	1	0
2	B	805	TTP	4	0
5	B	807	ATP	3	0
4	B	810	SO4	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, 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	715/792 (90%)	-0.46	2 (0%) 94 89	46, 61, 81, 110	2 (0%)
1	B	724/792 (91%)	-0.41	5 (0%) 89 79	46, 65, 94, 126	0
All	All	1439/1584 (90%)	-0.43	7 (0%) 91 84	46, 63, 90, 126	2 (0%)

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	444	CYS	6.6
1	A	218	CYS	6.3
1	B	107	PRO	2.6
1	B	676	LEU	2.3
1	B	659	ILE	2.2
1	B	33	PHE	2.2
1	B	108	HIS	2.1

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors

of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	SO4	B	813	5/5	0.93	0.27	2.20	70,70,72,72	0
4	SO4	A	812	5/5	0.96	0.21	0.04	83,83,85,86	0
4	SO4	B	810	5/5	0.97	0.13	-0.52	79,79,80,81	0
2	TTP	A	806	29/29	0.96	0.14	-1.04	59,63,74,75	0
2	TTP	B	805	29/29	0.97	0.13	-1.06	72,75,83,85	0
5	ATP	B	807	31/31	0.91	0.15	-1.57	65,69,76,76	0
3	MG	B	804	1/1	0.93	0.12	-	47,47,47,47	0
3	MG	B	802	1/1	0.96	0.10	-	62,62,62,62	0
4	SO4	B	811	5/5	0.94	0.13	-	99,100,100,100	0
4	SO4	A	809	5/5	0.89	0.13	-	127,127,127,127	0
3	MG	A	801	1/1	0.98	0.20	-	56,56,56,56	0
3	MG	B	803	1/1	0.94	0.19	-	42,42,42,42	0
4	SO4	A	808	5/5	0.94	0.16	-	86,87,87,87	0

6.5 Other polymers [i](#)

There are no such residues in this entry.