



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 19, 2016 – 06:38 PM GMT

PDB ID : 2BPO  
Title : CRYSTAL STRUCTURE OF THE YEAST CPR TRIPLE MUTANT: D74G, Y75F, K78A.  
Authors : Yermalitskaya, L.V.; Kim, Y.; Waterman, M.R.; Podust, L.M.  
Deposited on : 2005-04-21  
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 : 1.7.1 (RC1), CSD as537be (2016)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026982  
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) : rb-20026982

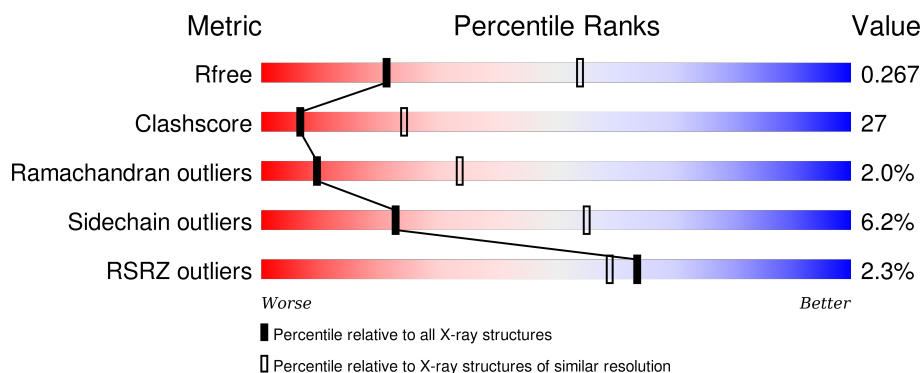
# 1 Overall quality at a glance

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	682	<div> <div></div> <div> <div></div> <div>49%</div> <div>42%</div> <div>6%</div> </div> </div>
1	B	682	<div> <div>3%</div> <div></div> <div>49%</div> <div>42%</div> <div>6%</div> </div>

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
5	SO4	A	761	-	-	-	X

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 10528 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.

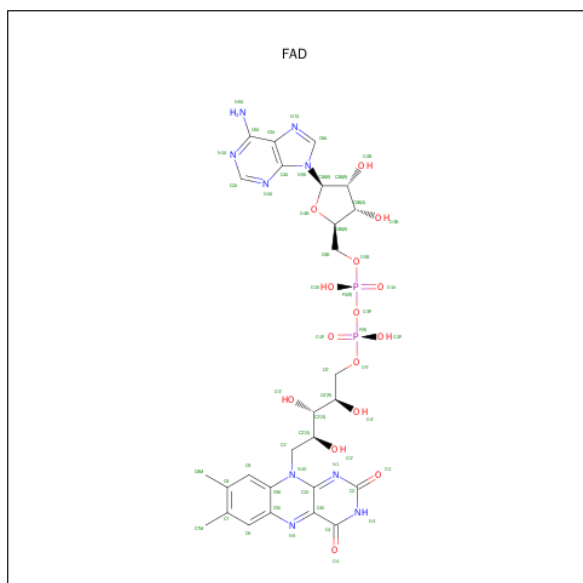
- Molecule 1 is a protein called NADPH-CYTOCHROM P450 REDUCTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	641	Total	C	N	O	S	0	0	0
			5040	3213	833	979	15			
1	B	641	Total	C	N	O	S	0	0	0
			5040	3213	833	979	15			

There are 6 discrepancies between the modelled and reference sequences:

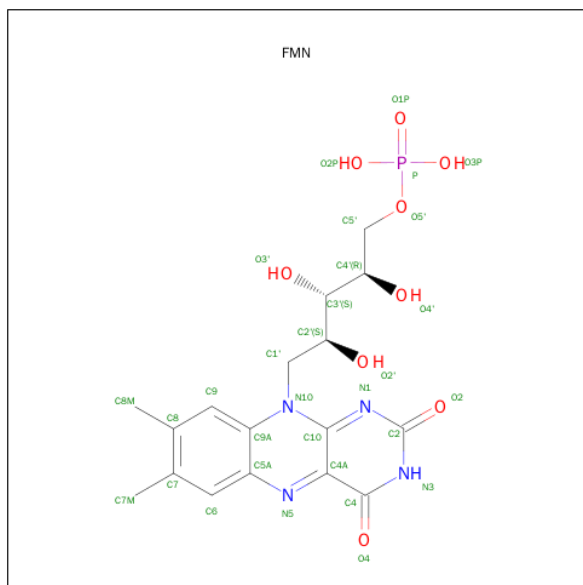
Chain	Residue	Modelled	Actual	Comment	Reference
A	74	GLY	ASP	ENGINEERED MUTATION	UNP P16603
A	75	PHE	TYR	ENGINEERED MUTATION	UNP P16603
A	78	ALA	LYS	ENGINEERED MUTATION	UNP P16603
B	74	GLY	ASP	ENGINEERED MUTATION	UNP P16603
B	75	PHE	TYR	ENGINEERED MUTATION	UNP P16603
B	78	ALA	LYS	ENGINEERED MUTATION	UNP P16603

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula:  $C_{27}H_{33}N_9O_{15}P_2$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

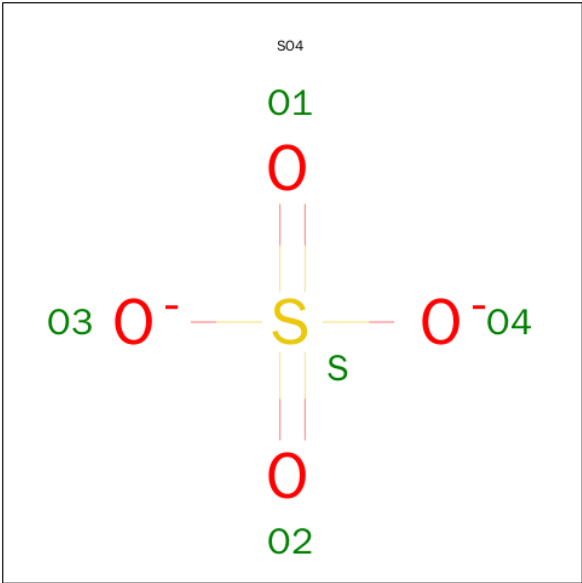
- Molecule 3 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula:  $C_{17}H_{21}N_4O_9P$ ).





Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			40	15	6	16	3		
4	B	1	Total	C	N	O	P	0	0
			40	15	6	16	3		

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



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

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

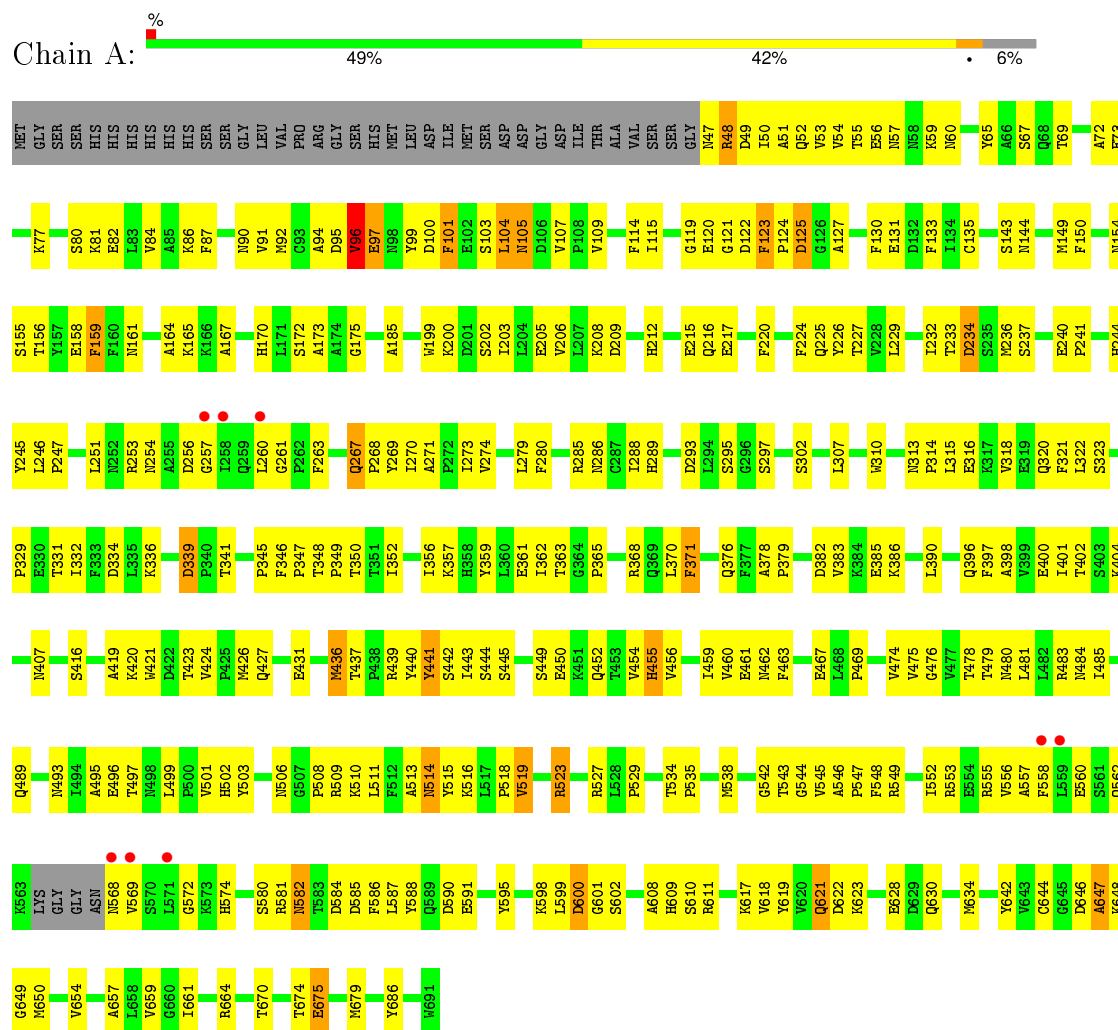
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	127	Total	O	0	0
			127	127		
6	B	58	Total	O	0	0
			58	58		

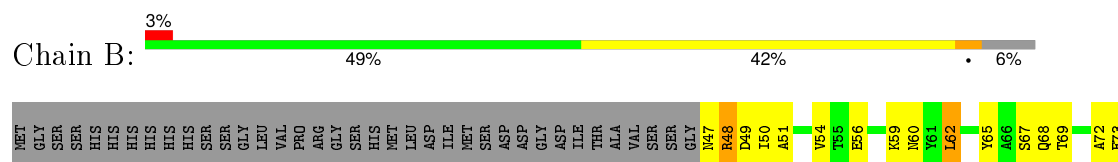
### 3 Residue-property plots

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: NADPH-CYTOCHROM P450 REDUCTASE



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K77	F159	Q259	D422	H502	S570	M650
S80	F160	L260	M426	Y503	L571	T656
K81	M161	G261	Q427	D504	H574	V659
E82	S80	P262	L505	N506	L575	O660
L83	K165	F263	P347	G507	L576	
V84	K166	D264	P349	P508	P577	
N90	A167	P268	V430	R509	L578	
V91	E168	Y269	T437	K510	S579	
N92	L179	I270	P438	L511	S580	
G93	L182	P272	I443	A513	R581	
A94	G188	I273	S444	S445	N582	
D95	G188	V274	S446	S447	T583	
V96	T191	S276	L448	L449	D584	
E97	T192	F280	S449	E450	F586	
N98	D193	R285	K451	R526	D590	
D100	E194	I288	Q452	L528	P591	
S103	D195	Y196	T453	P529	N592	
L104	M197	E291	H455	N531	P593	
V107	K200	L294	V460	P532	E594	
P108	I203	S297	F463	T534	M598	
V109	L204	N298	P464	V536	E604	
I110	E205	I210	E467	I539	V607	
S112	E210	L211	L468	G540	A608	
I113	L211	D305	P469	G542	H609	
E120	F220	V309	V475	V545	S610	
F123	P124	W310	Q476	A546	A611	
D125	G126	P311	W477	P547	T615	
G126	A127	P314	T478	F548	K616	
A127	N128	L315	T479	R549	V617	
N129	F130	E316	M480	G550	V618	
E131	D234	K317	L481	F551	V619	
T134	S235	V318	R483	I552	V620	
C135	N236	F321	M484	R553	D622	
L142	S237	L322	Q486	E554	L624	
L145	E240	I324	Q489	R555	K625	
R146	P241	P329	M490	V556	V627	
M149	L246	E330	M491	A557	E628	
L152	P247	T331	V492	F558	V631	
G153	H249	I332	M493	L559	G638	
N154	N252	D333	T494	E560	A639	
Y157	R253	K336	A495	K563	F640	
E158	G257	P337	T497	LYS	T641	
	I258	L338	M498	GLY	V642	
		D339	P499	ASN	V643	
			P500	N568	C644	
			V501	V569	A647	

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	78.36 Å 86.60 Å 259.72 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.18 – 2.90 50.00 – 2.89	Depositor EDS
% Data completeness (in resolution range)	87.2 (39.18-2.90) 86.9 (50.00-2.89)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.77 (at 2.91 Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.205 , 0.268 0.205 , 0.267	Depositor DCC
$R_{free}$ test set	3504 reflections (10.01%)	DCC
Wilson B-factor (Å <sup>2</sup> )	51.0	Xtriage
Anisotropy	0.708	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 57.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 37199 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	10528	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.76% 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: FMN, NAP, SO4, FAD

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	0.40	0/5156	0.65	1/7000 (0.0%)
1	B	0.38	0/5156	0.64	0/7000
All	All	0.39	0/10312	0.64	1/14000 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	407	ASN	N-CA-C	-5.18	97.02	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	441	TYR	Sidechain

### 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	5040	0	4933	259	0
1	B	5040	0	4933	297	0
2	A	53	0	31	2	0
2	B	53	0	31	4	0
3	A	31	0	19	2	0
3	B	31	0	19	1	0
4	A	40	0	19	2	0
4	B	40	0	19	2	0
5	A	10	0	0	0	0
5	B	5	0	0	0	0
6	A	127	0	0	9	0
6	B	58	0	0	8	0
All	All	10528	0	10004	556	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 27.

All (556) 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:B:619:TYR:HB3	1:B:621:GLN:HE22	1.03	1.12
1:B:621:GLN:H	1:B:621:GLN:NE2	1.54	1.06
1:B:539:ILE:HG23	1:B:620:VAL:HG11	1.39	1.03
1:B:621:GLN:N	1:B:621:GLN:HE21	1.57	1.01
1:B:625:LYS:O	1:B:628:GLU:HG3	1.60	1.00
1:B:582:ASN:HD21	1:B:584:ASP:HB2	1.27	0.99
1:B:582:ASN:ND2	1:B:584:ASP:H	1.60	0.99
1:A:621:GLN:HE21	1:A:621:GLN:N	1.62	0.98
1:B:445:SER:HB2	1:B:450:GLU:HG3	1.47	0.96
1:A:621:GLN:NE2	1:A:621:GLN:H	1.62	0.96
1:B:416:SER:HB2	1:B:419:ALA:HB3	1.49	0.94
1:B:225:GLN:HB3	1:B:336:LYS:HB2	1.50	0.93
1:A:67:SER:HB2	1:A:72:ALA:HB3	1.52	0.92
1:B:656:THR:O	1:B:659:VAL:HG12	1.68	0.91
1:B:60:ASN:HD22	1:B:90:ASN:H	1.01	0.91
1:B:621:GLN:H	1:B:621:GLN:HE21	0.91	0.90
1:A:60:ASN:ND2	1:A:90:ASN:H	1.68	0.90
1:B:427:GLN:H	1:B:427:GLN:HE21	1.14	0.89
1:B:619:TYR:HB3	1:B:621:GLN:NE2	1.87	0.88
1:B:427:GLN:H	1:B:427:GLN:NE2	1.70	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:110:ILE:HD12	1:B:211:LEU:HD21	1.58	0.86
1:B:619:TYR:CB	1:B:621:GLN:HE22	1.87	0.86
1:A:60:ASN:HD22	1:A:90:ASN:N	1.72	0.86
1:B:674:THR:HA	1:B:677:ILE:HD12	1.58	0.85
1:A:390:LEU:HD23	1:A:396:GLN:HG2	1.58	0.85
1:A:60:ASN:HD22	1:A:90:ASN:H	0.88	0.84
1:B:179:LEU:CD2	1:B:210:GLU:HG3	2.08	0.83
1:A:416:SER:HB3	1:A:419:ALA:HB3	1.60	0.83
1:A:361:GLU:HG2	1:A:436:MET:HA	1.61	0.83
1:A:105:ASN:HD21	1:A:144:ASN:H	1.23	0.83
1:B:234:ASP:HB3	1:B:247:PRO:HB2	1.59	0.82
1:A:227:THR:HB	6:A:2033:HOH:O	1.78	0.82
1:A:234:ASP:HB3	1:A:247:PRO:HB2	1.61	0.81
1:A:87:PHE:HE2	1:A:215:GLU:HG2	1.45	0.81
1:B:220:PHE:H	1:B:376:GLN:HE22	1.27	0.81
1:B:168:GLU:HG3	1:B:182:LEU:HD12	1.64	0.80
1:A:233:THR:HG22	1:A:234:ASP:N	1.96	0.80
1:B:451:LYS:O	1:B:452:GLN:HB2	1.81	0.80
1:B:310:TRP:HB2	1:B:518:PRO:HB2	1.64	0.80
1:B:60:ASN:ND2	1:B:90:ASN:H	1.78	0.79
1:B:237:SER:HA	1:B:246:LEU:HD21	1.63	0.79
1:A:225:GLN:HB3	1:A:336:LYS:HB3	1.66	0.79
1:B:60:ASN:HD22	1:B:90:ASN:N	1.79	0.78
1:A:600:ASP:CG	1:A:601:GLY:N	2.35	0.78
1:A:120:GLU:O	1:A:122:ASP:N	2.17	0.78
1:B:467:GLU:O	1:B:469:PRO:HD3	1.84	0.78
1:B:80:SER:O	1:B:84:VAL:HG23	1.83	0.78
1:B:179:LEU:HD21	1:B:210:GLU:HG3	1.66	0.77
1:A:600:ASP:CG	1:A:601:GLY:H	1.85	0.77
1:B:316:GLU:HG3	1:B:501:VAL:HG12	1.65	0.77
1:A:237:SER:HA	1:A:246:LEU:HD21	1.67	0.76
1:B:352:ILE:O	1:B:356:ILE:HG12	1.83	0.76
1:A:295:SER:HA	1:A:452:GLN:OE1	1.85	0.76
1:B:542:GLY:O	1:B:545:VAL:HG23	1.86	0.76
1:B:73:GLU:O	1:B:77:LYS:HG3	1.85	0.75
1:A:65:TYR:CZ	1:A:73:GLU:HG3	2.21	0.75
1:B:407:ASN:ND2	2:B:750:FAD:H61A	1.84	0.75
1:B:125:ASP:O	1:B:128:VAL:HG23	1.87	0.75
1:B:416:SER:HB2	1:B:419:ALA:CB	2.17	0.75
1:B:272:PRO:HB2	6:B:2022:HOH:O	1.86	0.75
1:A:232:ILE:HD12	1:A:236:MET:HB2	1.68	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:621:GLN:HE22	4:A:753:NAP:H2A	1.51	0.74
1:B:446:SER:O	1:B:450:GLU:HG2	1.86	0.74
1:B:233:THR:HG22	1:B:235:SER:H	1.50	0.74
1:A:549:ARG:O	1:A:553:ARG:HG3	1.88	0.74
1:B:352:ILE:HG12	1:B:426:MET:HE2	1.69	0.74
1:A:493:ASN:HD21	1:A:495:ALA:HB3	1.52	0.74
1:B:275:LYS:HB2	1:B:291:GLU:OE1	1.88	0.73
1:B:200:LYS:O	1:B:203:ILE:HG22	1.89	0.73
1:B:419:ALA:O	1:B:420:LYS:HB2	1.88	0.73
1:B:583:THR:HG23	6:B:2047:HOH:O	1.87	0.73
1:B:404:LYS:HG3	1:B:468:LEU:HD11	1.67	0.73
1:A:233:THR:HG22	1:A:234:ASP:H	1.54	0.73
1:A:87:PHE:CE2	1:A:215:GLU:HG2	2.22	0.73
1:A:310:TRP:HB2	1:A:518:PRO:HB2	1.71	0.72
1:A:269:TYR:CE1	1:A:297:SER:HB3	2.24	0.72
1:A:51:ALA:HB2	1:A:103:SER:O	1.89	0.72
1:B:142:LEU:HD13	1:B:145:LEU:HD12	1.72	0.72
1:B:647:ALA:O	1:B:650:MET:HB3	1.89	0.72
1:B:535:PRO:HB2	1:B:639:ALA:HB2	1.71	0.71
1:A:69:THR:HB	3:A:751:FMN:O2P	1.91	0.71
1:B:272:PRO:HG3	1:B:516:LYS:HE2	1.72	0.71
1:B:390:LEU:HD22	1:B:397:PHE:HA	1.72	0.70
1:A:523:ARG:HB2	1:A:523:ARG:HH11	1.55	0.70
1:B:274:VAL:HG12	1:B:275:LYS:HG3	1.71	0.69
1:A:82:GLU:OE1	1:A:200:LYS:HD2	1.91	0.69
1:A:48:ARG:HG2	1:A:100:ASP:OD2	1.93	0.68
1:A:493:ASN:HD22	1:A:496:GLU:HG3	1.57	0.68
1:A:439:ARG:HG3	1:A:478:THR:OG1	1.92	0.68
1:A:208:LYS:HE3	1:A:215:GLU:HG3	1.75	0.68
1:B:536:VAL:HB	1:B:574:HIS:ND1	2.09	0.68
1:B:274:VAL:HG23	6:B:2022:HOH:O	1.94	0.67
1:A:445:SER:HB3	1:A:455:HIS:CG	2.29	0.67
1:B:56:GLU:HG2	6:B:2001:HOH:O	1.94	0.67
1:B:513:ALA:O	1:B:514:ASN:HB2	1.94	0.67
1:A:322:LEU:HD13	1:A:329:PRO:HG3	1.77	0.67
1:A:621:GLN:H	1:A:621:GLN:HE21	0.80	0.67
1:B:556:VAL:O	1:B:560:GLU:HG3	1.94	0.67
1:B:197:MET:HE3	1:B:369:GLN:HB2	1.77	0.67
1:B:97:GLU:HG3	1:B:126:GLY:O	1.95	0.66
1:B:123:PHE:HD2	1:B:123:PHE:N	1.93	0.66
1:A:123:PHE:CZ	1:A:167:ALA:HB2	2.30	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:531:ASN:HD22	1:B:532:PRO:HD2	1.60	0.66
1:A:582:ASN:ND2	1:A:584:ASP:H	1.94	0.66
1:A:670:THR:O	1:A:674:THR:HG23	1.96	0.66
1:A:558:PHE:CE2	1:A:569:VAL:HG21	2.31	0.65
1:A:493:ASN:ND2	1:A:495:ALA:HB3	2.11	0.65
1:A:475:VAL:HB	1:A:480:ASN:ND2	2.12	0.65
1:B:110:ILE:CD1	1:B:211:LEU:HD21	2.25	0.65
1:A:390:LEU:CD2	1:A:396:GLN:HG2	2.27	0.65
1:B:547:PRO:HG2	1:B:644:CYS:SG	2.37	0.65
1:B:552:ILE:HD12	1:B:592:TRP:HZ3	1.60	0.65
1:B:617:LYS:HD3	1:B:619:TYR:CZ	2.32	0.64
1:B:562:GLN:HG2	1:B:569:VAL:HG22	1.79	0.64
1:B:558:PHE:HZ	1:B:569:VAL:HG11	1.62	0.64
1:B:50:ILE:HG23	1:B:51:ALA:N	2.12	0.64
1:A:513:ALA:O	1:A:514:ASN:HB2	1.97	0.64
1:B:484:ASN:ND2	1:B:503:TYR:H	1.95	0.64
1:A:461:GLU:OE2	4:A:753:NAP:H1D	1.98	0.64
1:B:448:LEU:HD23	1:B:448:LEU:O	1.98	0.64
1:A:445:SER:HB3	1:A:455:HIS:ND1	2.13	0.63
1:A:273:ILE:O	1:A:489:GLN:NE2	2.31	0.63
1:B:314:PRO:O	1:B:318:VAL:HG23	1.98	0.63
1:B:437:THR:HG22	1:B:438:PRO:O	1.98	0.63
1:B:582:ASN:HD21	1:B:584:ASP:CB	2.09	0.63
1:B:123:PHE:CD2	1:B:123:PHE:N	2.66	0.63
1:B:545:VAL:HG21	1:B:578:TYR:CE1	2.34	0.63
1:B:485:ILE:HG12	1:B:505:LEU:CD1	2.29	0.63
1:A:368:ARG:HB2	6:A:2026:HOH:O	1.97	0.63
1:B:460:VAL:HA	1:B:479:THR:HB	1.80	0.63
1:B:145:LEU:HD23	1:B:146:ARG:N	2.14	0.62
1:B:659:VAL:CB	1:B:677:ILE:HD11	2.29	0.62
1:B:220:PHE:H	1:B:376:GLN:NE2	1.97	0.62
1:B:451:LYS:O	1:B:452:GLN:CB	2.48	0.62
1:B:236:MET:CE	1:B:332:ILE:HG21	2.29	0.62
1:A:382:ASP:OD1	1:A:386:LYS:HE3	1.99	0.62
1:B:581:ARG:HB2	1:B:585:ASP:OD2	1.99	0.62
1:B:47:ASN:O	1:B:49:ASP:N	2.32	0.62
1:B:448:LEU:HD22	1:B:557:ALA:HB1	1.81	0.62
1:B:529:PRO:HD3	1:B:642:TYR:OH	2.00	0.62
1:A:307:LEU:HD21	1:A:519:VAL:HG21	1.80	0.61
1:B:59:LYS:HD3	1:B:90:ASN:OD1	2.00	0.61
1:A:47:ASN:N	1:A:52:GLN:HE21	1.98	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:355:ALA:HA	1:B:359:TYR:CD1	2.36	0.61
1:B:135:CYS:SG	1:B:166:LYS:HE2	2.40	0.61
1:A:123:PHE:HD1	1:A:123:PHE:N	1.98	0.61
1:B:82:GLU:OE1	1:B:200:LYS:HD2	2.01	0.61
1:A:123:PHE:CD1	1:A:123:PHE:N	2.69	0.61
1:B:580:SER:HB2	1:B:585:ASP:OD1	2.01	0.61
1:B:355:ALA:HA	1:B:359:TYR:HD1	1.64	0.61
1:B:386:LYS:NZ	6:B:2031:HOH:O	2.31	0.61
1:A:233:THR:CG2	1:A:234:ASP:N	2.64	0.60
1:A:274:VAL:HG11	1:A:293:ASP:HB2	1.82	0.60
1:B:497:THR:HG22	1:B:498:ASN:H	1.65	0.60
1:A:314:PRO:O	1:A:318:VAL:HG23	2.00	0.60
1:B:400:GLU:O	1:B:401:ILE:HD13	2.01	0.60
1:A:523:ARG:CB	1:A:523:ARG:HH11	2.14	0.60
1:A:253:ARG:HD3	1:A:257:GLY:O	2.01	0.60
1:A:50:ILE:HG23	1:A:51:ALA:N	2.15	0.60
1:A:315:LEU:HD12	1:A:502:HIS:CD2	2.36	0.60
1:A:288:ILE:HD12	1:A:288:ILE:N	2.17	0.60
1:A:135:CYS:HA	1:A:170:HIS:ND1	2.16	0.60
1:A:572:GLY:O	1:A:574:HIS:HD2	1.85	0.59
1:A:581:ARG:HD3	1:A:611:ARG:HD2	1.84	0.59
1:B:447:SER:O	1:B:451:LYS:HG3	2.02	0.59
1:A:484:ASN:ND2	1:A:502:HIS:HA	2.18	0.59
1:A:158:GLU:O	1:A:159:PHE:HB2	2.02	0.59
1:A:546:ALA:HB3	1:A:547:PRO:HD3	1.84	0.59
1:A:123:PHE:HZ	1:A:167:ALA:HB2	1.67	0.59
1:B:113:ILE:O	1:B:149:MET:HB2	2.02	0.59
1:A:233:THR:CG2	1:A:234:ASP:H	2.16	0.59
1:A:623:LYS:HA	1:A:623:LYS:HE2	1.84	0.59
1:A:232:ILE:HA	1:A:236:MET:HE2	1.85	0.58
1:B:558:PHE:CZ	1:B:569:VAL:HG11	2.38	0.58
1:B:592:TRP:HB2	1:B:593:PRO:HD3	1.85	0.58
1:B:531:ASN:HD22	1:B:532:PRO:CD	2.17	0.58
1:B:437:THR:HG23	1:B:438:PRO:HD2	1.84	0.58
1:B:285:ARG:HD3	1:B:581:ARG:NH1	2.19	0.58
1:A:398:ALA:HA	1:A:402:THR:HB	1.85	0.58
1:B:145:LEU:HD23	1:B:146:ARG:H	1.66	0.58
1:A:334:ASP:HB3	6:A:2033:HOH:O	2.03	0.58
1:B:352:ILE:HG23	1:B:426:MET:HE1	1.85	0.57
1:A:244:HIS:H	1:A:244:HIS:CD2	2.21	0.57
1:A:400:GLU:C	1:A:401:ILE:HD12	2.25	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:50:ILE:HG23	1:B:51:ALA:H	1.67	0.57
1:B:485:ILE:HG12	1:B:505:LEU:HD11	1.87	0.57
1:B:364:GLY:H	1:B:407:ASN:ND2	2.03	0.57
1:A:232:ILE:HD12	1:A:236:MET:HE2	1.86	0.57
1:A:209:ASP:O	1:A:212:HIS:HD2	1.88	0.57
1:A:443:ILE:HG23	1:A:454:VAL:HG13	1.86	0.57
1:B:370:LEU:O	1:B:370:LEU:HD23	2.04	0.57
1:A:547:PRO:HG2	1:A:644:CYS:SG	2.45	0.57
1:B:448:LEU:HB2	1:B:554:GLU:CD	2.24	0.57
1:B:315:LEU:HG	1:B:502:HIS:O	2.05	0.56
1:B:179:LEU:HD23	1:B:210:GLU:HG3	1.85	0.56
1:B:582:ASN:ND2	1:B:584:ASP:N	2.43	0.56
1:A:232:ILE:HA	1:A:236:MET:CE	2.35	0.56
1:B:236:MET:HE1	1:B:332:ILE:HG21	1.87	0.56
1:B:371:PHE:CE2	1:B:415:LEU:HD11	2.40	0.56
1:A:105:ASN:ND2	1:A:144:ASN:HB2	2.21	0.56
1:A:236:MET:HE1	1:A:332:ILE:HG21	1.87	0.56
1:B:375:ILE:HD11	1:B:388:THR:HA	1.87	0.56
1:B:309:VAL:O	1:B:311:PRO:HD3	2.05	0.56
1:A:552:ILE:O	1:A:556:VAL:HG23	2.05	0.56
1:A:314:PRO:HG3	1:A:503:TYR:CE2	2.41	0.56
1:A:630:GLN:O	1:A:634:MET:HG3	2.06	0.56
1:B:157:TYR:CE1	1:B:690:VAL:HG23	2.41	0.55
1:B:194:GLU:OE2	1:B:368:ARG:NH1	2.39	0.55
1:B:484:ASN:HD22	1:B:503:TYR:H	1.54	0.55
1:B:535:PRO:HB2	1:B:639:ALA:CB	2.37	0.55
1:B:580:SER:O	1:B:609:HIS:HA	2.07	0.55
1:B:51:ALA:HB2	1:B:103:SER:O	2.06	0.55
1:A:245:TYR:HE1	1:A:267:GLN:NE2	2.05	0.55
1:B:407:ASN:HD21	2:B:750:FAD:H61A	1.54	0.55
1:B:154:ASN:ND2	1:B:188:GLY:CA	2.69	0.55
1:A:254:ASN:HB3	1:A:260:LEU:HD11	1.87	0.55
1:B:263:PHE:CD2	1:B:269:TYR:HB2	2.42	0.54
1:B:291:GLU:OE2	1:B:455:HIS:NE2	2.40	0.54
1:A:313:ASN:ND2	6:A:2050:HOH:O	2.40	0.54
1:B:234:ASP:CB	1:B:247:PRO:HB2	2.34	0.54
1:A:199:TRP:CZ2	1:A:203:ILE:HG13	2.43	0.54
1:A:379:PRO:HD3	1:A:421:TRP:CE3	2.42	0.54
1:B:263:PHE:CE2	1:B:269:TYR:HB2	2.43	0.54
1:B:161:ASN:OD1	1:B:164:ALA:HB3	2.08	0.54
1:B:443:ILE:HG23	1:B:454:VAL:HG13	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:220:PHE:N	1:B:376:GLN:HE22	2.03	0.54
1:A:379:PRO:HD2	1:A:383:VAL:HG11	1.90	0.54
1:A:582:ASN:HD22	1:A:584:ASP:H	1.55	0.53
1:A:657:ALA:O	1:A:661:ILE:HG13	2.09	0.53
1:B:674:THR:HA	1:B:677:ILE:CD1	2.35	0.53
1:B:404:LYS:CG	1:B:468:LEU:HD11	2.38	0.53
1:B:542:GLY:O	1:B:545:VAL:CG2	2.56	0.53
1:B:369:GLN:NE2	1:B:369:GLN:O	2.42	0.53
1:A:400:GLU:O	1:A:404:LYS:HD2	2.09	0.53
1:B:659:VAL:HG23	1:B:677:ILE:HD11	1.89	0.53
1:A:675:GLU:O	1:A:679:MET:HG3	2.09	0.53
1:A:97:GLU:HA	6:A:2011:HOH:O	2.09	0.53
1:B:182:LEU:HD23	1:B:182:LEU:C	2.30	0.53
1:A:159:PHE:N	1:A:159:PHE:CD1	2.76	0.53
1:A:562:GLN:HG3	1:A:569:VAL:HG22	1.91	0.53
1:B:659:VAL:HG21	1:B:674:THR:OG1	2.09	0.52
1:B:476:GLY:HA3	2:B:750:FAD:O2P	2.08	0.52
1:A:608:ALA:HB2	1:A:623:LYS:HG3	1.91	0.52
1:A:591:GLU:HB3	1:A:595:TYR:CE1	2.45	0.52
1:B:577:PHE:HB3	1:B:620:VAL:HG13	1.91	0.52
1:A:232:ILE:CD1	1:A:236:MET:HB2	2.39	0.52
1:A:159:PHE:N	1:A:159:PHE:HD1	2.07	0.52
1:A:476:GLY:HA3	2:A:750:FAD:O2P	2.09	0.52
1:A:401:ILE:HD12	1:A:401:ILE:N	2.24	0.52
1:B:475:VAL:HB	1:B:480:ASN:ND2	2.24	0.52
1:A:331:THR:HB	1:A:352:ILE:HD12	1.92	0.52
1:A:321:PHE:HD2	1:A:356:ILE:HD13	1.74	0.52
1:A:94:ALA:HB1	1:A:99:TYR:CE1	2.45	0.52
1:B:445:SER:HB3	1:B:455:HIS:CG	2.44	0.52
1:A:268:PRO:HD3	1:A:310:TRP:CH2	2.44	0.51
1:A:154:ASN:OD1	1:A:156:THR:HB	2.09	0.51
1:A:587:LEU:HA	6:A:2042:HOH:O	2.09	0.51
1:B:225:GLN:HA	6:B:2019:HOH:O	2.09	0.51
1:B:548:PHE:HA	1:B:551:PHE:HB2	1.92	0.51
1:A:423:THR:HG22	1:A:423:THR:O	2.10	0.51
1:B:621:GLN:HA	1:B:624:LEU:HD12	1.92	0.51
1:A:444:SER:HA	1:A:546:ALA:O	2.11	0.51
1:A:86:LYS:O	1:A:216:GLN:HG2	2.10	0.51
1:B:498:ASN:O	1:B:499:LEU:C	2.49	0.51
1:A:467:GLU:O	1:A:469:PRO:HD3	2.10	0.51
1:B:322:LEU:HD13	1:B:329:PRO:HG3	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:677:ILE:O	1:B:680:LEU:N	2.43	0.51
1:B:419:ALA:O	1:B:420:LYS:CB	2.58	0.51
1:A:599:LEU:O	1:A:600:ASP:OD1	2.29	0.51
1:B:316:GLU:CG	1:B:501:VAL:HG12	2.36	0.51
1:B:197:MET:HE2	1:B:197:MET:HA	1.93	0.51
1:A:316:GLU:O	1:A:320:GLN:HG3	2.11	0.51
1:B:673:ALA:O	1:B:677:ILE:HG13	2.10	0.51
1:A:236:MET:HE1	1:A:332:ILE:HD13	1.92	0.51
1:A:513:ALA:O	1:A:516:LYS:HD2	2.10	0.51
1:B:371:PHE:CZ	1:B:415:LEU:HD11	2.46	0.50
1:B:107:VAL:HG12	1:B:109:VAL:H	1.77	0.50
1:A:346:PHE:HB2	1:A:347:PRO:CD	2.41	0.50
1:A:241:PRO:HB3	1:A:268:PRO:HG3	1.92	0.50
1:A:50:ILE:HG23	1:A:51:ALA:H	1.76	0.50
1:B:379:PRO:HD2	1:B:383:VAL:HG11	1.93	0.50
1:A:286:ASN:O	1:A:460:VAL:HG23	2.12	0.50
1:B:67:SER:HB2	1:B:72:ALA:HB3	1.94	0.50
1:B:404:LYS:HB3	1:B:406:PHE:CE2	2.46	0.50
1:B:123:PHE:H	1:B:123:PHE:HD2	1.59	0.50
1:A:288:ILE:HG12	1:A:483:ARG:HA	1.91	0.50
1:B:348:THR:HA	1:B:349:PRO:C	2.32	0.50
1:B:380:ASN:ND2	1:B:383:VAL:H	2.09	0.50
1:B:337:PRO:HB3	1:B:342:VAL:O	2.12	0.50
1:B:288:ILE:HD12	1:B:486:GLN:HG3	1.94	0.50
1:A:628:GLU:OE2	1:A:664:ARG:NH1	2.45	0.50
1:A:279:LEU:CD1	1:A:289:HIS:HB2	2.42	0.50
1:B:94:ALA:HB1	1:B:99:TYR:CE1	2.46	0.50
1:B:576:LEU:HD23	1:B:577:PHE:N	2.27	0.49
1:B:123:PHE:CD1	1:B:131:GLU:HB2	2.47	0.49
1:A:348:THR:HA	1:A:349:PRO:C	2.32	0.49
1:B:314:PRO:HG3	1:B:503:TYR:CZ	2.47	0.49
1:B:48:ARG:HH11	1:B:48:ARG:HG2	1.76	0.49
1:B:497:THR:HG22	1:B:498:ASN:N	2.26	0.49
1:A:560:GLU:OE2	1:A:598:LYS:HD3	2.12	0.49
1:A:279:LEU:HD11	1:A:289:HIS:HB2	1.95	0.49
1:B:607:VAL:O	1:B:623:LYS:HE3	2.12	0.49
1:A:523:ARG:HB2	1:A:523:ARG:NH1	2.26	0.49
1:B:369:GLN:C	1:B:369:GLN:NE2	2.66	0.49
1:A:356:ILE:HG23	1:A:362:ILE:HG21	1.95	0.49
1:A:499:LEU:HG	1:A:501:VAL:O	2.12	0.49
1:A:229:LEU:HD21	6:A:2033:HOH:O	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:310:TRP:CD1	1:A:310:TRP:N	2.80	0.49
1:B:607:VAL:HG12	1:B:608:ALA:N	2.26	0.49
1:A:101:PHE:O	1:A:133:PHE:CZ	2.66	0.49
1:B:445:SER:HB3	1:B:455:HIS:ND1	2.27	0.49
1:B:395:ASP:O	1:B:399:VAL:HG23	2.11	0.49
1:A:610:SER:HB2	1:A:617:LYS:HG3	1.95	0.49
1:A:443:ILE:HG22	1:A:445:SER:H	1.78	0.49
1:A:555:ARG:HE	1:A:574:HIS:HE1	1.59	0.49
1:A:316:GLU:HG3	1:A:501:VAL:HG12	1.94	0.49
1:B:51:ALA:HB3	1:B:103:SER:OG	2.13	0.49
1:A:421:TRP:O	1:A:424:VAL:HG23	2.12	0.49
1:B:627:TYR:O	1:B:631:VAL:HG23	2.13	0.48
1:A:460:VAL:HA	1:A:479:THR:HB	1.94	0.48
1:A:237:SER:O	1:A:350:THR:HA	2.14	0.48
1:A:542:GLY:C	1:A:544:GLY:H	2.16	0.48
1:B:638:GLY:HA2	1:B:685:ARG:CZ	2.42	0.48
1:A:427:GLN:O	1:A:431:GLU:HG3	2.13	0.48
1:A:582:ASN:HD22	1:A:582:ASN:C	2.17	0.48
1:A:220:PHE:HB2	1:A:376:GLN:HE22	1.77	0.48
1:A:463:PHE:CE1	1:A:474:VAL:HB	2.49	0.48
1:A:69:THR:HG22	1:A:69:THR:O	2.13	0.48
1:B:315:LEU:HG	1:B:503:TYR:HA	1.95	0.48
1:B:346:PHE:HB2	1:B:347:PRO:CD	2.44	0.48
1:A:150:PHE:CZ	1:A:185:ALA:HB2	2.49	0.48
1:B:426:MET:N	1:B:427:GLN:HE21	2.12	0.48
1:B:269:TYR:CE2	1:B:297:SER:HB3	2.49	0.48
1:A:365:PRO:HG3	2:A:750:FAD:C2A	2.43	0.48
1:A:450:GLU:HG2	1:A:455:HIS:CE1	2.49	0.48
1:A:347:PRO:HD2	1:A:359:TYR:CZ	2.48	0.48
1:B:96:VAL:HG21	1:B:130:PHE:CD2	2.48	0.48
1:B:352:ILE:HG23	1:B:426:MET:CE	2.44	0.48
1:B:618:VAL:HG11	1:B:623:LYS:HE2	1.95	0.48
1:B:446:SER:HB2	1:B:554:GLU:OE2	2.12	0.48
1:B:65:TYR:CZ	1:B:73:GLU:HG3	2.49	0.48
1:A:322:LEU:CD1	1:A:329:PRO:HG3	2.44	0.48
1:B:161:ASN:OD1	1:B:161:ASN:O	2.32	0.48
1:B:321:PHE:O	1:B:324:ILE:HG22	2.14	0.48
1:B:59:LYS:CD	1:B:90:ASN:OD1	2.62	0.48
1:B:444:SER:HA	1:B:546:ALA:O	2.14	0.47
1:B:104:LEU:HD23	1:B:142:LEU:HD13	1.96	0.47
1:B:154:ASN:HD21	1:B:188:GLY:CA	2.27	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:441:TYR:HB3	1:A:456:VAL:HG13	1.96	0.47
1:B:260:LEU:HA	1:B:298:ASN:OD1	2.13	0.47
1:A:245:TYR:CE1	1:A:267:GLN:NE2	2.83	0.47
1:B:659:VAL:HB	1:B:677:ILE:HD11	1.95	0.47
1:B:399:VAL:O	1:B:404:LYS:HE3	2.14	0.47
1:A:271:ALA:O	1:A:516:LYS:HA	2.12	0.47
1:A:323:SER:O	1:A:420:LYS:HD3	2.15	0.47
1:A:599:LEU:O	1:A:602:SER:HB2	2.15	0.47
1:B:288:ILE:HD11	1:B:483:ARG:HG3	1.95	0.47
1:B:448:LEU:HD22	1:B:557:ALA:CB	2.45	0.47
1:A:442:SER:HB3	1:A:547:PRO:HG3	1.96	0.47
1:A:274:VAL:CG1	1:A:293:ASP:HB2	2.44	0.47
1:B:152:LEU:N	1:B:152:LEU:HD12	2.29	0.47
1:B:406:PHE:HB3	1:B:410:ASP:HB2	1.97	0.47
1:B:280:PHE:CD2	1:B:585:ASP:HA	2.50	0.47
1:B:608:ALA:HB2	1:B:623:LYS:HG3	1.97	0.47
1:B:509:ARG:HG2	1:B:509:ARG:HH11	1.79	0.47
1:B:331:THR:HB	1:B:352:ILE:HD12	1.97	0.47
1:A:542:GLY:O	1:A:545:VAL:HG12	2.15	0.47
1:B:421:TRP:N	1:B:421:TRP:CD1	2.83	0.47
1:B:268:PRO:HB3	1:B:310:TRP:CE2	2.50	0.46
1:B:285:ARG:HH21	1:B:585:ASP:CG	2.18	0.46
1:A:124:PRO:O	1:A:125:ASP:C	2.53	0.46
1:B:448:LEU:HB2	1:B:554:GLU:OE1	2.16	0.46
1:B:659:VAL:HA	1:B:677:ILE:HD11	1.96	0.46
1:B:294:LEU:HD11	1:B:454:VAL:HG21	1.97	0.46
1:B:659:VAL:CA	1:B:677:ILE:HD11	2.46	0.46
1:A:59:LYS:HD3	1:A:90:ASN:ND2	2.31	0.46
1:A:493:ASN:ND2	1:A:496:GLU:HG3	2.28	0.46
1:B:285:ARG:HH21	1:B:585:ASP:CB	2.28	0.46
1:A:357:LYS:O	1:A:357:LYS:HG2	2.15	0.46
1:A:321:PHE:CD2	1:A:356:ILE:HD13	2.51	0.46
1:B:400:GLU:HA	1:B:404:LYS:HE3	1.96	0.46
1:A:52:GLN:HG3	1:A:56:GLU:OE2	2.15	0.46
1:B:380:ASN:ND2	1:B:382:ASP:HB2	2.31	0.46
1:B:426:MET:O	1:B:430:VAL:HG23	2.15	0.46
1:B:96:VAL:HG21	1:B:130:PHE:CG	2.51	0.46
1:B:192:THR:HB	6:B:2014:HOH:O	2.15	0.46
1:B:91:VAL:HG12	1:B:92:MET:N	2.31	0.46
1:B:559:LEU:HD22	1:B:599:LEU:HD23	1.98	0.46
1:B:503:TYR:CD1	1:B:503:TYR:N	2.84	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:202:SER:O	1:A:206:VAL:HG23	2.15	0.46
1:B:659:VAL:CG2	1:B:677:ILE:HD11	2.45	0.46
1:B:233:THR:CG2	1:B:234:ASP:N	2.79	0.46
1:B:503:TYR:O	1:B:505:LEU:HD23	2.15	0.46
1:B:154:ASN:HB3	1:B:157:TYR:HD2	1.80	0.46
1:B:545:VAL:HG21	1:B:578:TYR:CD1	2.49	0.46
1:B:529:PRO:HG3	1:B:640:PHE:CG	2.51	0.46
1:B:608:ALA:HB1	1:B:618:VAL:HG12	1.98	0.46
1:A:619:TYR:O	1:A:622:ASP:HB2	2.16	0.46
1:A:51:ALA:O	1:A:55:THR:HG23	2.16	0.45
1:A:493:ASN:HB3	1:A:496:GLU:HG3	1.99	0.45
1:A:172:SER:OG	1:A:173:ALA:N	2.49	0.45
1:A:143:SER:HA	1:A:175:GLY:O	2.17	0.45
1:B:539:ILE:HD13	1:B:624:LEU:HD11	1.97	0.45
1:A:556:VAL:O	1:A:560:GLU:HG3	2.17	0.45
1:A:650:MET:O	1:A:654:VAL:HG23	2.16	0.45
1:A:115:ILE:HG21	1:A:164:ALA:HA	1.99	0.45
1:A:580:SER:O	1:A:609:HIS:HA	2.16	0.45
1:A:279:LEU:HD21	1:A:588:TYR:CZ	2.51	0.45
1:A:647:ALA:O	1:A:650:MET:HB2	2.17	0.45
1:B:627:TYR:O	1:B:628:GLU:C	2.55	0.45
1:B:48:ARG:HB3	1:B:100:ASP:OD2	2.15	0.45
1:A:538:MET:HB3	1:A:548:PHE:CD2	2.52	0.45
1:B:541:PRO:HG3	1:B:620:VAL:HG21	1.99	0.45
1:B:62:LEU:HD13	1:B:111:VAL:HG13	1.99	0.45
1:A:77:LYS:O	1:A:81:LYS:HD3	2.17	0.45
1:B:81:LYS:HG3	6:B:2035:HOH:O	2.16	0.45
1:A:370:LEU:O	1:A:370:LEU:HD13	2.17	0.45
1:B:54:VAL:HG13	1:B:59:LYS:HB2	1.99	0.44
1:A:270:ILE:HD12	1:A:511:LEU:HD22	1.99	0.44
1:A:53:VAL:O	1:A:57:ASN:ND2	2.51	0.44
1:A:107:VAL:HG12	1:A:109:VAL:HG22	1.98	0.44
1:A:280:PHE:CD2	1:A:585:ASP:HA	2.52	0.44
1:B:677:ILE:HA	1:B:680:LEU:HD12	1.98	0.44
1:B:246:LEU:HB2	1:B:249:HIS:HD2	1.82	0.44
1:A:260:LEU:HB3	1:A:261:GLY:H	1.61	0.44
1:A:95:ASP:O	1:A:97:GLU:N	2.51	0.44
1:B:611:ARG:NE	4:B:753:NAP:O2X	2.49	0.44
1:A:288:ILE:HD13	1:A:460:VAL:HG22	2.00	0.44
1:A:385:GLU:HA	1:A:385:GLU:OE1	2.16	0.44
1:A:205:GLU:HA	1:A:205:GLU:OE1	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:680:LEU:HB3	1:B:686:TYR:HB2	2.00	0.44
1:A:244:HIS:CD2	1:A:267:GLN:HG2	2.53	0.44
1:B:154:ASN:ND2	1:B:188:GLY:N	2.66	0.44
1:A:237:SER:CA	1:A:246:LEU:HD21	2.41	0.44
1:B:236:MET:HG2	1:B:349:PRO:HB2	2.00	0.44
1:A:302:SER:HB2	1:A:527:ARG:NH2	2.32	0.44
1:B:232:ILE:HG22	1:B:233:THR:N	2.33	0.44
1:A:123:PHE:H	1:A:123:PHE:HD1	1.61	0.44
1:A:314:PRO:HG3	1:A:503:TYR:CZ	2.52	0.44
1:A:608:ALA:HB1	1:A:618:VAL:HG12	1.99	0.44
1:B:305:ASP:OD1	1:B:527:ARG:NH2	2.46	0.44
1:A:80:SER:O	1:A:84:VAL:HG23	2.18	0.44
1:A:154:ASN:HB2	3:A:751:FMN:H1'1	1.99	0.44
1:B:314:PRO:HG3	1:B:503:TYR:CE2	2.53	0.44
1:A:484:ASN:HD22	1:A:503:TYR:HD1	1.66	0.44
1:A:423:THR:HB	6:A:2068:HOH:O	2.17	0.44
1:A:506:ASN:O	1:A:510:LYS:HA	2.18	0.44
1:B:513:ALA:O	1:B:514:ASN:CB	2.63	0.43
1:A:628:GLU:CD	1:A:664:ARG:HH11	2.21	0.43
1:A:114:PHE:CD2	1:A:150:PHE:HB3	2.53	0.43
1:B:159:PHE:CD1	1:B:159:PHE:N	2.86	0.43
1:A:263:PHE:CD2	1:A:269:TYR:HB2	2.53	0.43
1:B:437:THR:CG2	1:B:438:PRO:N	2.81	0.43
1:A:95:ASP:C	1:A:95:ASP:OD2	2.56	0.43
1:B:607:VAL:CG1	1:B:608:ALA:N	2.81	0.43
1:B:492:VAL:O	1:B:494:ILE:N	2.51	0.43
1:A:449:SER:HB3	1:A:557:ALA:HB2	2.00	0.43
1:B:483:ARG:HH12	1:B:498:ASN:HB2	1.83	0.43
1:A:485:ILE:HG23	1:A:515:TYR:HB3	1.99	0.43
1:A:54:VAL:HG13	1:A:59:LYS:HB2	2.00	0.43
1:A:49:ASP:O	1:A:52:GLN:HB3	2.18	0.43
1:A:253:ARG:HG2	1:A:253:ARG:HH11	1.83	0.43
1:B:628:GLU:O	1:B:631:VAL:HB	2.18	0.43
1:A:508:PRO:O	1:A:509:ARG:C	2.57	0.43
1:B:233:THR:HG22	1:B:234:ASP:N	2.33	0.43
1:A:455:HIS:N	1:A:455:HIS:ND1	2.67	0.43
1:B:273:ILE:O	1:B:489:GLN:NE2	2.46	0.43
1:B:610:SER:HB2	1:B:617:LYS:HE2	2.00	0.43
1:A:295:SER:C	1:A:297:SER:H	2.22	0.43
1:A:65:TYR:CE1	1:A:73:GLU:HG3	2.53	0.43
1:A:50:ILE:CG2	1:A:51:ALA:N	2.80	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:619:TYR:CB	1:B:621:GLN:NE2	2.62	0.43
1:A:400:GLU:CB	1:A:401:ILE:HD12	2.49	0.43
1:B:83:LEU:HA	1:B:83:LEU:HD12	1.85	0.43
1:B:437:THR:HG23	1:B:438:PRO:CD	2.46	0.42
1:A:104:LEU:O	1:A:107:VAL:HG23	2.19	0.42
1:B:69:THR:HB	3:B:751:FMN:O2P	2.19	0.42
1:A:558:PHE:CZ	1:A:569:VAL:HG21	2.54	0.42
1:A:161:ASN:O	1:A:165:LYS:HG3	2.18	0.42
1:B:507:GLY:HA3	1:B:512:PHE:CD1	2.54	0.42
1:A:378:ALA:HA	1:A:379:PRO:HD3	1.87	0.42
1:A:647:ALA:O	1:A:648:LYS:C	2.56	0.42
1:B:463:PHE:HA	1:B:464:PRO:HD3	1.85	0.42
1:B:443:ILE:HG22	1:B:445:SER:H	1.84	0.42
1:B:499:LEU:HA	1:B:499:LEU:HD23	1.77	0.42
1:B:546:ALA:HB3	1:B:547:PRO:HD3	2.00	0.42
1:B:558:PHE:CZ	1:B:562:GLN:NE2	2.88	0.42
1:B:271:ALA:O	1:B:516:LYS:HA	2.19	0.42
1:B:446:SER:HB3	1:B:550:GLY:O	2.18	0.42
1:B:276:SER:O	1:B:490:ASN:ND2	2.46	0.42
1:B:237:SER:CA	1:B:246:LEU:HD21	2.42	0.42
1:B:65:TYR:CE1	1:B:95:ASP:HA	2.54	0.42
1:A:199:TRP:CE2	1:A:203:ILE:HG13	2.55	0.42
1:B:448:LEU:HB2	1:B:554:GLU:OE2	2.19	0.42
1:B:659:VAL:CG1	1:B:660:GLY:N	2.83	0.42
1:A:95:ASP:C	1:A:97:GLU:H	2.23	0.42
1:A:226:TYR:CD1	1:A:427:GLN:HG2	2.55	0.42
1:B:575:ILE:HA	1:B:604:GLU:O	2.20	0.42
1:B:193:ASP:O	1:B:196:TYR:HB3	2.20	0.42
1:B:446:SER:C	1:B:450:GLU:HG2	2.39	0.41
1:A:368:ARG:HG3	1:A:397:PHE:CG	2.55	0.41
1:B:373:SER:HB3	1:B:428:PHE:HZ	1.84	0.41
1:A:105:ASN:HD21	1:A:144:ASN:N	2.03	0.41
1:A:513:ALA:O	1:A:516:LYS:CD	2.67	0.41
1:B:334:ASP:HB2	1:B:349:PRO:HG3	2.02	0.41
1:B:380:ASN:HD21	1:B:382:ASP:HB2	1.84	0.41
1:B:511:LEU:HA	1:B:511:LEU:HD23	1.90	0.41
1:A:49:ASP:HB3	1:A:52:GLN:HB3	2.01	0.41
1:A:534:THR:HA	1:A:535:PRO:HD3	1.97	0.41
1:B:510:LYS:O	1:B:513:ALA:HB2	2.20	0.41
1:A:481:LEU:HA	1:A:503:TYR:CE1	2.55	0.41
1:B:302:SER:HB2	1:B:527:ARG:HH21	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:594:GLU:O	1:B:598:LYS:HG2	2.19	0.41
1:B:390:LEU:CD2	1:B:397:PHE:HA	2.44	0.41
1:A:96:VAL:HG13	1:A:130:PHE:HB2	2.02	0.41
1:A:60:ASN:ND2	1:A:90:ASN:HB3	2.36	0.41
1:A:659:VAL:HG11	1:A:674:THR:CG2	2.50	0.41
1:B:493:ASN:ND2	1:B:496:GLU:HG3	2.35	0.41
1:A:224:PHE:CZ	1:A:345:PRO:HD3	2.56	0.41
1:B:448:LEU:HD23	1:B:448:LEU:C	2.41	0.41
1:A:307:LEU:HG	1:A:519:VAL:HG22	2.02	0.41
1:B:478:THR:N	2:B:750:FAD:O1P	2.52	0.41
1:A:96:VAL:HG22	1:A:130:PHE:CD1	2.55	0.41
1:B:241:PRO:HB3	1:B:268:PRO:HG3	2.03	0.41
1:A:154:ASN:C	1:A:156:THR:H	2.24	0.41
1:B:558:PHE:CE1	1:B:569:VAL:HG21	2.56	0.41
1:B:50:ILE:CG2	1:B:51:ALA:N	2.80	0.41
1:A:368:ARG:O	1:A:371:PHE:HB2	2.19	0.41
1:A:484:ASN:ND2	1:A:503:TYR:H	2.19	0.41
1:A:288:ILE:HD13	1:A:460:VAL:CG2	2.50	0.41
1:A:288:ILE:N	1:A:288:ILE:CD1	2.83	0.41
1:A:279:LEU:HD23	1:A:587:LEU:HD22	2.03	0.41
1:B:62:LEU:HD23	1:B:92:MET:HB3	2.03	0.41
1:A:339:ASP:OD1	1:A:341:THR:N	2.53	0.41
1:B:253:ARG:HG2	1:B:259:GLN:HA	2.02	0.41
1:A:268:PRO:HB3	1:A:310:TRP:CE2	2.56	0.41
1:B:104:LEU:HD23	1:B:142:LEU:CD1	2.51	0.41
1:B:531:ASN:ND2	1:B:532:PRO:HD2	2.29	0.41
1:A:216:GLN:O	1:A:217:GLU:C	2.59	0.41
1:A:240:GLU:HG2	1:A:245:TYR:O	2.21	0.40
1:A:542:GLY:C	1:A:544:GLY:N	2.73	0.40
1:B:691:TRP:CZ3	4:B:753:NAP:H3D	2.56	0.40
1:A:529:PRO:HD3	1:A:642:TYR:OH	2.20	0.40
1:A:131:GLU:CD	6:A:2012:HOH:O	2.59	0.40
1:B:49:ASP:C	1:B:49:ASP:OD1	2.59	0.40
1:A:556:VAL:HG21	1:A:595:TYR:HD2	1.85	0.40
1:A:646:ASP:O	1:A:647:ALA:C	2.59	0.40
1:B:556:VAL:HA	1:B:599:LEU:HD21	2.02	0.40
1:B:154:ASN:ND2	1:B:188:GLY:HA3	2.36	0.40
1:A:440:TYR:CD1	1:A:440:TYR:N	2.88	0.40
1:A:156:THR:HG23	1:A:649:GLY:H	1.86	0.40
1:B:534:THR:HG21	1:B:640:PHE:CE1	2.56	0.40
1:A:91:VAL:HG12	1:A:92:MET:N	2.35	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:157:TYR:HE1	1:B:690:VAL:HG23	1.83	0.40
1:B:48:ARG:NH1	1:B:48:ARG:HG2	2.37	0.40
1:A:251:LEU:HA	1:A:251:LEU:HD23	1.95	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	637/682 (93%)	568 (89%)	59 (9%)	10 (2%)	12	40
1	B	637/682 (93%)	561 (88%)	60 (9%)	16 (2%)	7	27
All	All	1274/1364 (93%)	1129 (89%)	119 (9%)	26 (2%)	9	33

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	121	GLY
1	B	48	ARG
1	A	96	VAL
1	A	647	ALA
1	B	493	ASN
1	B	669	THR
1	A	155	SER
1	A	497	THR
1	A	514	ASN
1	B	120	GLU
1	B	420	LYS
1	B	452	GLN
1	B	514	ASN
1	B	526	PHE
1	A	127	ALA

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Mol	Chain	Res	Type
1	A	543	THR
1	B	261	GLY
1	B	451	LYS
1	B	571	LEU
1	A	101	PHE
1	A	119	GLY
1	B	158	GLU
1	B	422	ASP
1	B	124	PRO
1	B	499	LEU
1	B	569	VAL

### 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	557/590 (94%)	525 (94%)	32 (6%)	25	59
1	B	557/590 (94%)	520 (93%)	37 (7%)	21	51
All	All	1114/1180 (94%)	1045 (94%)	69 (6%)	23	55

All (69) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	48	ARG
1	A	96	VAL
1	A	97	GLU
1	A	104	LEU
1	A	105	ASN
1	A	123	PHE
1	A	125	ASP
1	A	149	MET
1	A	159	PHE
1	A	234	ASP
1	A	256	ASP
1	A	267	GLN

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Mol	Chain	Res	Type
1	A	285	ARG
1	A	339	ASP
1	A	363	THR
1	A	371	PHE
1	A	426	MET
1	A	436	MET
1	A	437	THR
1	A	455	HIS
1	A	459	ILE
1	A	462	ASN
1	A	519	VAL
1	A	523	ARG
1	A	568	ASN
1	A	582	ASN
1	A	586	PHE
1	A	590	ASP
1	A	600	ASP
1	A	621	GLN
1	A	675	GLU
1	A	686	TYR
1	B	62	LEU
1	B	68	GLN
1	B	96	VAL
1	B	123	PHE
1	B	134	ILE
1	B	145	LEU
1	B	154	ASN
1	B	159	PHE
1	B	191	THR
1	B	205	GLU
1	B	221	THR
1	B	240	GLU
1	B	252	ASN
1	B	264	ASP
1	B	316	GLU
1	B	339	ASP
1	B	369	GLN
1	B	371	PHE
1	B	389	LEU
1	B	404	LYS
1	B	426	MET
1	B	427	GLN

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Mol	Chain	Res	Type
1	B	481	LEU
1	B	499	LEU
1	B	514	ASN
1	B	526	PHE
1	B	530	SER
1	B	545	VAL
1	B	555	ARG
1	B	569	VAL
1	B	586	PHE
1	B	590	ASP
1	B	615	THR
1	B	621	GLN
1	B	650	MET
1	B	671	ASP
1	B	686	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (45) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	60	ASN
1	A	105	ASN
1	A	212	HIS
1	A	216	GLN
1	A	225	GLN
1	A	244	HIS
1	A	250	GLN
1	A	252	ASN
1	A	267	GLN
1	A	286	ASN
1	A	313	ASN
1	A	380	ASN
1	A	480	ASN
1	A	484	ASN
1	A	493	ASN
1	A	502	HIS
1	A	562	GLN
1	A	574	HIS
1	A	582	ASN
1	A	621	GLN
1	A	630	GLN
1	B	60	ASN
1	B	98	ASN

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Mol	Chain	Res	Type
1	B	144	ASN
1	B	148	ASN
1	B	154	ASN
1	B	249	HIS
1	B	286	ASN
1	B	306	HIS
1	B	320	GLN
1	B	369	GLN
1	B	376	GLN
1	B	380	ASN
1	B	407	ASN
1	B	427	GLN
1	B	452	GLN
1	B	480	ASN
1	B	484	ASN
1	B	486	GLN
1	B	493	ASN
1	B	498	ASN
1	B	531	ASN
1	B	562	GLN
1	B	582	ASN
1	B	621	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

9 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$
2	FAD	A	750	-	52,58,58	1.65	6 (11%)	52,89,89	2.21	5 (9%)
3	FMN	A	751	-	32,33,33	1.81	7 (21%)	34,50,50	3.50	9 (26%)
4	NAP	A	753	-	37,43,52	1.34	6 (16%)	45,67,80	2.17	8 (17%)
5	SO4	A	760	-	4,4,4	0.21	0	6,6,6	0.11	0
5	SO4	A	761	-	4,4,4	0.22	0	6,6,6	0.05	0
2	FAD	B	750	-	52,58,58	1.73	8 (15%)	52,89,89	2.16	5 (9%)
3	FMN	B	751	-	32,33,33	1.90	6 (18%)	34,50,50	3.36	11 (32%)
4	NAP	B	753	-	37,43,52	1.27	4 (10%)	45,67,80	2.13	5 (11%)
5	SO4	B	762	-	4,4,4	0.19	0	6,6,6	0.11	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	FAD	A	750	-	-	0/30/50/50	0/6/6/6
3	FMN	A	751	-	-	0/18/18/18	0/3/3/3
4	NAP	A	753	-	-	0/23/59/67	0/4/4/5
5	SO4	A	760	-	-	0/0/0/0	0/0/0/0
5	SO4	A	761	-	-	0/0/0/0	0/0/0/0
2	FAD	B	750	-	-	0/30/50/50	0/6/6/6
3	FMN	B	751	-	-	0/18/18/18	0/3/3/3
4	NAP	B	753	-	-	0/23/59/67	0/4/4/5
5	SO4	B	762	-	-	0/0/0/0	0/0/0/0

All (37) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	753	NAP	C2B-C1B	-3.18	1.44	1.53
4	B	753	NAP	C2B-C1B	-2.86	1.45	1.53
4	A	753	NAP	P2B-O2X	-2.58	1.45	1.54
4	B	753	NAP	P2B-O2X	-2.39	1.46	1.54
4	A	753	NAP	C5A-N7A	-2.33	1.31	1.39
3	B	751	FMN	P-O2P	-2.30	1.46	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	751	FMN	P-O2P	-2.30	1.46	1.54
2	A	750	FAD	C5A-C4A	-2.25	1.35	1.40
3	A	751	FMN	P-O3P	-2.18	1.47	1.54
2	B	750	FAD	C5A-C4A	-2.10	1.35	1.40
2	B	750	FAD	O4B-C1B	2.10	1.44	1.41
2	A	750	FAD	C4A-N3A	2.20	1.38	1.35
3	A	751	FMN	C5A-N5	2.37	1.39	1.35
4	A	753	NAP	O4B-C1B	2.40	1.44	1.41
3	A	751	FMN	C9A-N10	2.41	1.42	1.38
2	B	750	FAD	C9-C8	2.41	1.44	1.37
2	A	750	FAD	C5X-N5	2.42	1.39	1.35
4	B	753	NAP	O4D-C1D	2.47	1.46	1.41
3	B	751	FMN	C5A-N5	2.75	1.39	1.35
4	A	753	NAP	O4D-C1D	2.77	1.47	1.41
4	A	753	NAP	C4A-N3A	3.17	1.40	1.35
2	B	750	FAD	C4A-N3A	3.31	1.40	1.35
2	B	750	FAD	C5X-N5	3.36	1.40	1.35
4	B	753	NAP	C4A-N3A	3.41	1.40	1.35
3	B	751	FMN	C9A-N10	3.47	1.43	1.38
3	B	751	FMN	C4A-N5	3.49	1.38	1.33
3	A	751	FMN	C4A-N5	3.99	1.39	1.33
3	B	751	FMN	C4-N3	4.06	1.40	1.33
2	A	750	FAD	C4-N3	4.44	1.41	1.33
2	B	750	FAD	C4-N3	4.50	1.41	1.33
3	A	751	FMN	C4-N3	4.75	1.41	1.33
2	A	750	FAD	C9A-N10	5.11	1.46	1.38
3	A	751	FMN	C10-N10	5.17	1.45	1.39
2	B	750	FAD	C9A-N10	5.29	1.46	1.38
2	B	750	FAD	C4X-N5	5.79	1.42	1.33
2	A	750	FAD	C4X-N5	6.04	1.42	1.33
3	B	751	FMN	C10-N10	6.13	1.46	1.39

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	753	NAP	N3A-C2A-N1A	-9.85	121.13	128.87
4	B	753	NAP	N3A-C2A-N1A	-9.31	121.56	128.87
3	A	751	FMN	N3-C2-N1	-7.53	115.01	127.69
4	B	753	NAP	C1B-N9A-C4A	-7.41	118.53	126.81
3	B	751	FMN	N3-C2-N1	-7.13	115.69	127.69
4	A	753	NAP	C1B-N9A-C4A	-6.89	119.11	126.81
2	A	750	FAD	C4X-C4-N3	-6.48	115.05	123.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	751	FMN	C4A-C4-N3	-6.36	115.21	123.52
2	B	750	FAD	C4X-C4-N3	-6.20	115.42	123.52
3	B	751	FMN	C4A-C4-N3	-6.08	115.58	123.52
3	A	751	FMN	C4A-C10-N10	-5.31	116.66	120.52
3	A	751	FMN	C4-C4A-C10	-5.29	116.56	119.94
3	B	751	FMN	C4-C4A-C10	-5.07	116.70	119.94
2	A	750	FAD	N3-C2-N1	-5.01	119.26	127.69
2	B	750	FAD	N3-C2-N1	-5.00	119.27	127.69
3	B	751	FMN	C4A-C10-N10	-4.55	117.22	120.52
3	A	751	FMN	C4A-N5-C5A	-3.26	112.88	116.72
3	B	751	FMN	C4A-N5-C5A	-3.14	113.02	116.72
4	A	753	NAP	O2X-P2B-O2B	-2.68	98.62	106.62
4	A	753	NAP	O4B-C1B-C2B	-2.52	102.06	106.60
4	B	753	NAP	O2X-P2B-O2B	-2.44	99.33	106.62
3	A	751	FMN	O5'-P-O1P	-2.41	101.03	107.08
3	B	751	FMN	C6-C5A-N5	-2.38	115.95	118.92
2	A	750	FAD	C4-C4X-C10	-2.25	118.50	119.94
3	B	751	FMN	C4-C4A-N5	-2.22	116.00	118.70
3	B	751	FMN	O5'-P-O1P	-2.20	101.55	107.08
4	A	753	NAP	O3B-C3B-C4B	-2.04	104.91	111.01
4	A	753	NAP	C2A-N1A-C6A	2.01	122.35	118.77
4	A	753	NAP	C4B-O4B-C1B	2.05	111.81	109.64
4	B	753	NAP	O2X-P2B-O1X	2.10	117.47	110.63
2	B	750	FAD	O2B-C2B-C3B	2.12	118.71	111.86
3	A	751	FMN	O3P-P-O2P	2.50	116.63	107.44
3	B	751	FMN	O3P-P-O2P	2.51	116.65	107.44
3	A	751	FMN	C9A-C5A-N5	2.59	126.39	122.18
3	B	751	FMN	C9A-C5A-N5	2.68	126.54	122.18
4	A	753	NAP	P2B-O2B-C2B	2.72	128.53	121.56
4	B	753	NAP	P2B-O2B-C2B	3.04	129.34	121.56
2	A	750	FAD	C1'-N10-C9A	3.51	122.90	118.83
2	B	750	FAD	C1'-N10-C9A	4.17	123.67	118.83
2	B	750	FAD	C4-N3-C2	11.60	124.84	115.16
2	A	750	FAD	C4-N3-C2	11.79	125.00	115.16
3	B	751	FMN	C4-N3-C2	13.94	126.79	115.16
3	A	751	FMN	C4-N3-C2	14.42	127.19	115.16

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	750	FAD	2	0
3	A	751	FMN	2	0
4	A	753	NAP	2	0
2	B	750	FAD	4	0
3	B	751	FMN	1	0
4	B	753	NAP	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, 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	641/682 (93%)	0.07	8 (1%) 81 78	30, 50, 74, 99	0
1	B	641/682 (93%)	0.24	21 (3%) 50 42	33, 60, 81, 105	0
All	All	1282/1364 (93%)	0.15	29 (2%) 64 59	30, 55, 78, 105	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	669	THR	3.9
1	A	559	LEU	3.7
1	B	468	LEU	3.6
1	A	260	LEU	3.5
1	B	569	VAL	3.3
1	B	674	THR	3.2
1	B	231	GLU	3.0
1	A	568	ASN	2.7
1	B	382	ASP	2.7
1	B	513	ALA	2.6
1	A	569	VAL	2.6
1	B	388	THR	2.6
1	B	489	GLN	2.6
1	B	663	SER	2.6
1	B	257	GLY	2.5
1	B	258	ILE	2.5
1	B	668	ILE	2.5
1	B	675	GLU	2.4
1	B	125	ASP	2.4
1	B	515	TYR	2.3
1	A	258	ILE	2.3
1	A	571	LEU	2.2
1	A	558	PHE	2.2
1	B	511	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	230	ASN	2.1
1	A	257	GLY	2.0
1	B	659	VAL	2.0
1	B	531	ASN	2.0
1	B	492	VAL	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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
5	SO4	A	761	5/5	0.89	0.26	2.93	128,129,129,129	0
2	FAD	B	750	53/53	0.96	0.21	0.61	42,50,56,60	0
4	NAP	A	753	40/48	0.97	0.20	0.36	32,41,77,78	0
4	NAP	B	753	40/48	0.91	0.20	0.15	94,99,114,114	0
5	SO4	A	760	5/5	0.93	0.17	-0.17	87,87,89,89	0
2	FAD	A	750	53/53	0.97	0.18	-0.29	23,31,36,38	0
3	FMN	A	751	31/31	0.96	0.18	-0.38	37,41,45,47	0
3	FMN	B	751	31/31	0.94	0.17	-0.58	58,64,66,67	0
5	SO4	B	762	5/5	0.77	0.17	-	144,144,144,144	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.