



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 10:35 am GMT

PDB ID : 1FLL  
Title : MOLECULAR BASIS FOR CD40 SIGNALING MEDIATED BY TRAF3  
Authors : Ni, C.-Z.; Welsh, K.; Leo, E.; Chiou, C.-K.; Wu, H.; Reed, J.C.; Ely, K.R.  
Deposited on : 2000-08-14  
Resolution : 3.50 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  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
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) : recalc28949

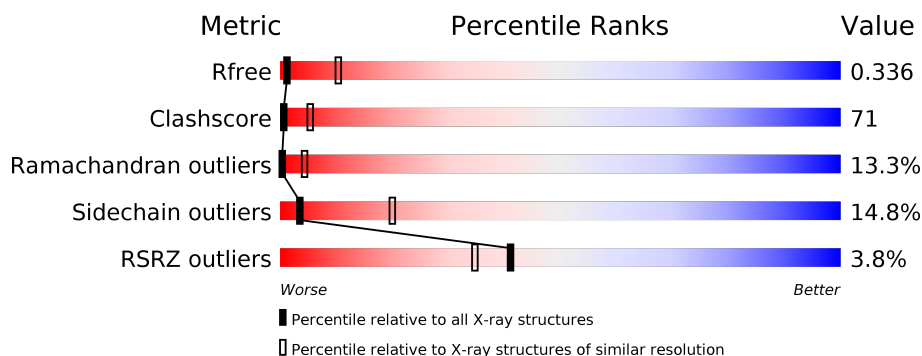
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.50 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))
$R_{free}$	100719	1195 (3.60-3.40)
Clashscore	112137	1322 (3.60-3.40)
Ramachandran outliers	110173	1283 (3.60-3.40)
Sidechain outliers	110143	1284 (3.60-3.40)
RSRZ outliers	101464	1226 (3.60-3.40)

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	228	<div> <div>2%</div> <div> <div>21%</div> <div>55%</div> <div>13%</div> <div>10%</div> </div> </div>
1	B	228	<div> <div>2%</div> <div> <div>19%</div> <div>55%</div> <div>16%</div> <div>10%</div> </div> </div>
2	X	21	<div> <div>14%</div> <div> <div>19%</div> <div>52%</div> <div>24%</div> <div>5%</div> </div> </div>
2	Y	21	<div> <div>19%</div> <div> <div>19%</div> <div>62%</div> <div>10%</div> <div>10%</div> </div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3558 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 TNF RECEPTOR ASSOCIATED FACTOR 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	205	Total	C	N	O	S	0	0	0
			1626	1035	277	303	11			
1	B	205	Total	C	N	O	S	0	0	0
			1626	1035	277	303	11			

- Molecule 2 is a protein called B-CELL SURFACE ANTIGEN CD40.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	X	21	Total	C	N	O	0	0	0
			153	92	27	34			
2	Y	21	Total	C	N	O	0	0	0
			153	92	27	34			

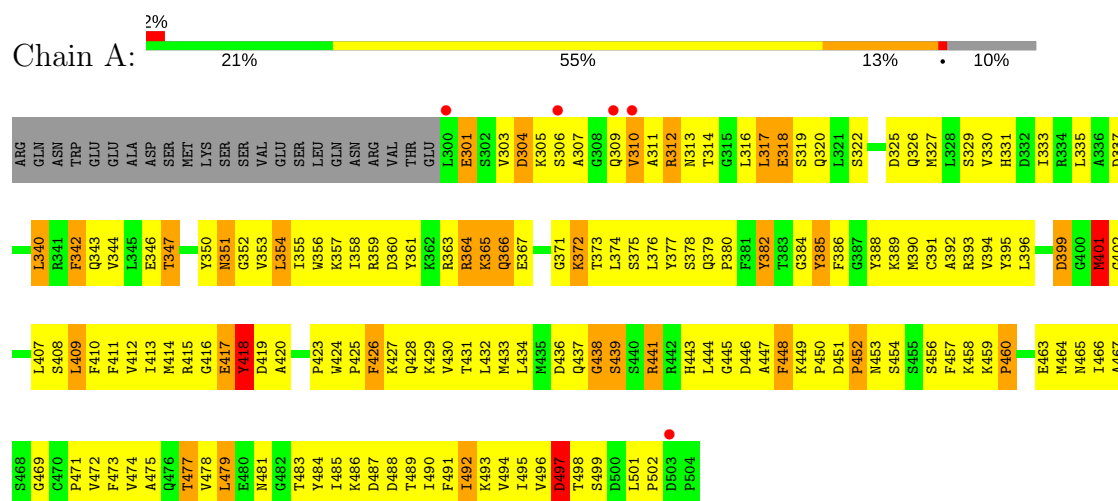
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
X	246	LYS	ASN	ENGINEERED	UNP P25942
X	258	SER	CYS	ENGINEERED	UNP P25942
Y	246	LYS	ASN	ENGINEERED	UNP P25942
Y	258	SER	CYS	ENGINEERED	UNP P25942

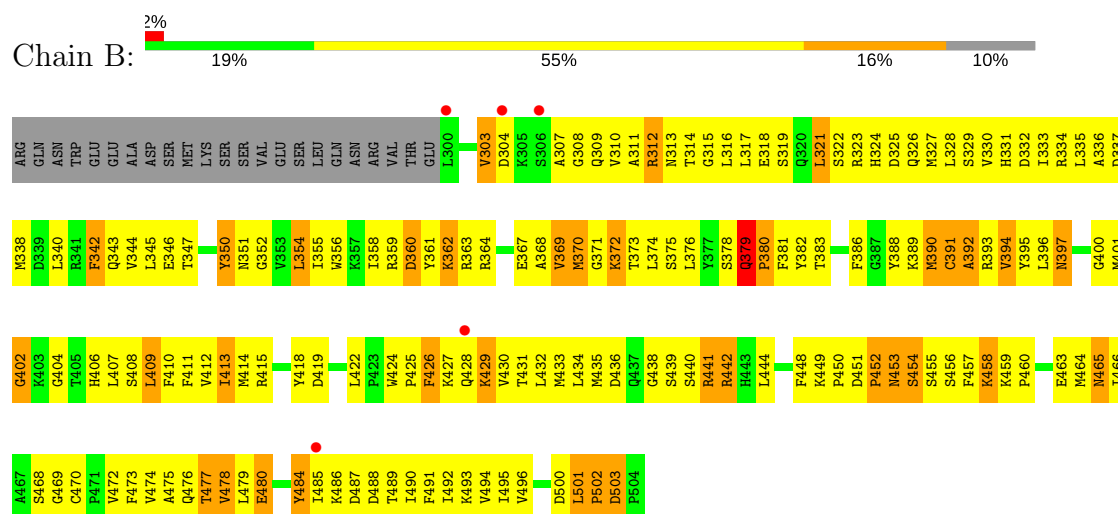
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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.

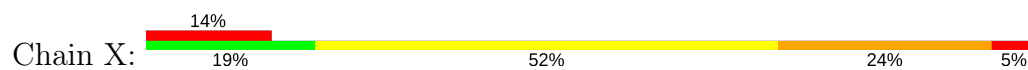
#### • Molecule 1: TNF RECEPTOR ASSOCIATED FACTOR 3

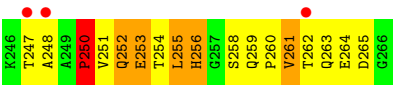


#### • Molecule 1: TNF RECEPTOR ASSOCIATED FACTOR 3

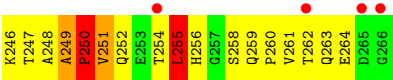


#### • Molecule 2: B-CELL SURFACE ANTIGEN CD40





● Molecule 2: B-CELL SURFACE ANTIGEN CD40



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 3 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	83.76Å 83.76Å 212.57Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	8.00 – 3.50 41.88 – 3.50	Depositor EDS
% Data completeness (in resolution range)	72.6 (8.00-3.50) 81.9 (41.88-3.50)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.44 (at 3.48Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.173 , 0.312 0.231 , 0.336	Depositor DCC
$R_{free}$ test set	432 reflections (4.58%)	DCC
Wilson B-factor (Å <sup>2</sup> )	56.7	Xtriage
Anisotropy	0.980	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 35.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.398 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.85	EDS
Total number of atoms	3558	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.20% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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	0.39	0/1661	0.72	0/2239
1	B	0.42	0/1661	0.71	0/2239
2	X	0.52	0/155	0.78	0/211
2	Y	0.67	0/155	0.81	0/211
All	All	0.42	0/3632	0.72	0/4900

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
2	X	0	1
All	All	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	388	TYR	Sidechain
2	X	264	GLU	Peptide

### 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	1626	0	1622	237	0
1	B	1626	0	1622	234	0
2	X	153	0	144	25	0
2	Y	153	0	144	26	0
All	All	3558	0	3532	504	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 71.

All (504) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:254:THR:OG1	2:X:265:ASP:HB2	1.40	1.19
1:A:466:ILE:HG23	2:X:253:GLU:HB2	1.37	1.07
1:B:312:ARG:HA	1:B:312:ARG:HE	1.24	1.02
2:X:252:GLN:N	2:X:252:GLN:HE21	1.59	1.00
1:B:410:PHE:HA	1:B:469:GLY:HA3	1.45	0.96
2:X:254:THR:OG1	2:X:265:ASP:CB	2.13	0.95
1:A:367:GLU:HB3	1:A:373:THR:HB	1.50	0.92
1:B:397:ASN:ND2	1:B:404:GLY:HA2	1.84	0.92
1:A:326:GLN:O	1:A:330:VAL:HG23	1.70	0.91
1:B:332:ASP:O	1:B:336:ALA:HB2	1.72	0.90
1:B:501:LEU:HD22	1:B:502:PRO:HD2	1.56	0.88
1:A:364:ARG:HG2	1:A:376:LEU:HD11	1.55	0.87
1:A:395:TYR:HD1	1:A:410:PHE:HE1	1.18	0.86
1:A:306:SER:HA	1:A:309:GLN:HE21	1.38	0.86
1:A:375:SER:HB3	1:A:395:TYR:CE2	2.10	0.86
1:A:436:ASP:OD2	1:A:441:ARG:HG3	1.76	0.85
1:B:427:LYS:HA	1:B:450:PRO:HB2	1.57	0.85
2:X:259:GLN:HB3	2:X:260:PRO:HD2	1.57	0.85
1:B:322:SER:HA	1:B:325:ASP:HB2	1.59	0.84
1:A:391:CYS:HB2	1:A:414:MET:SD	2.17	0.84
1:B:397:ASN:HD21	1:B:404:GLY:HA2	1.42	0.83
1:B:354:LEU:O	1:B:493:LYS:HA	1.79	0.82
1:B:309:GLN:HE21	1:B:312:ARG:HG3	1.43	0.82
1:B:424:TRP:HB3	1:B:425:PRO:HA	1.60	0.82
1:A:354:LEU:HD23	1:A:355:ILE:H	1.44	0.81
2:Y:249:ALA:HB1	2:Y:250:PRO:CD	2.11	0.81
1:A:429:LYS:HB3	1:A:497:ASP:CB	2.10	0.81
2:Y:249:ALA:HB1	2:Y:250:PRO:HD2	1.62	0.81
1:A:408:SER:HB3	1:A:471:PRO:HA	1.61	0.80
1:B:493:LYS:HE2	1:B:495:ILE:HG12	1.62	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:331:HIS:HA	1:B:334:ARG:HB2	1.62	0.80
1:B:356:TRP:HB3	1:B:492:ILE:HB	1.63	0.80
1:A:352:GLY:O	1:A:353:VAL:HG23	1.80	0.80
1:A:466:ILE:HG23	2:X:253:GLU:CB	2.12	0.79
1:B:383:THR:HG22	1:B:496:VAL:HG11	1.65	0.78
1:A:451:ASP:HB2	2:X:248:ALA:O	1.84	0.78
1:B:355:ILE:HA	1:B:492:ILE:O	1.84	0.77
1:B:402:GLY:O	1:B:406:HIS:HB2	1.85	0.77
1:A:424:TRP:HE3	1:A:425:PRO:HA	1.49	0.77
1:B:468:SER:HB2	2:Y:252:GLN:HG3	1.65	0.77
1:B:448:PHE:HD1	1:B:449:LYS:N	1.84	0.76
1:B:317:LEU:O	1:B:321:LEU:HB2	1.85	0.76
1:A:375:SER:CB	1:A:393:ARG:HE	1.99	0.75
1:A:396:LEU:HA	1:A:407:LEU:HG	1.68	0.75
1:B:441:ARG:HH11	1:B:441:ARG:HB3	1.51	0.75
1:A:303:VAL:O	1:A:306:SER:HB3	1.85	0.75
1:A:317:LEU:H	1:A:317:LEU:HD22	1.52	0.75
1:A:425:PRO:HB2	1:A:457:PHE:O	1.87	0.75
1:A:350:TYR:HD2	1:A:384:GLY:O	1.69	0.75
1:A:429:LYS:HB3	1:A:497:ASP:HB3	1.68	0.75
1:B:468:SER:HA	2:Y:252:GLN:HA	1.68	0.75
1:B:441:ARG:HB3	1:B:441:ARG:NH1	2.02	0.75
1:A:412:VAL:HG12	1:A:413:ILE:N	2.02	0.74
1:B:434:LEU:HB3	1:B:444:LEU:HB2	1.68	0.74
1:B:442:ARG:H	1:B:442:ARG:HD3	1.51	0.74
1:A:484:TYR:O	1:A:490:ILE:HG22	1.88	0.73
1:B:376:LEU:HB2	1:B:394:VAL:HG12	1.70	0.73
1:A:382:TYR:HB2	1:A:384:GLY:O	1.88	0.72
1:B:354:LEU:HD12	1:B:494:VAL:HG23	1.71	0.72
1:A:466:ILE:CG2	2:X:253:GLU:HB2	2.18	0.72
1:A:306:SER:HA	1:A:309:GLN:NE2	2.04	0.71
1:B:312:ARG:NE	1:B:312:ARG:HA	2.03	0.71
1:B:364:ARG:O	1:B:396:LEU:HD12	1.88	0.71
1:B:391:CYS:HB2	1:B:414:MET:SD	2.31	0.71
1:B:407:LEU:HB3	1:B:474:VAL:HB	1.73	0.71
1:A:354:LEU:HD23	1:A:355:ILE:N	2.06	0.71
1:A:350:TYR:CE2	1:A:385:TYR:HA	2.26	0.71
1:A:426:PHE:HE1	1:A:428:GLN:HB2	1.56	0.70
1:A:407:LEU:HD13	1:A:479:LEU:HD22	1.72	0.70
1:B:355:ILE:HD13	1:B:493:LYS:HB2	1.72	0.70
1:B:391:CYS:HB3	1:B:412:VAL:HB	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:456:SER:HA	1:B:466:ILE:HB	1.73	0.70
1:A:395:TYR:CD1	1:A:410:PHE:HE1	2.07	0.69
1:A:412:VAL:HG12	1:A:413:ILE:H	1.56	0.69
1:A:449:LYS:O	2:X:248:ALA:HB3	1.92	0.69
1:A:386:PHE:HB3	1:A:418:TYR:CD2	2.27	0.69
1:A:359:ARG:HB3	1:A:489:THR:HG22	1.72	0.69
2:Y:254:THR:O	2:Y:255:LEU:HB2	1.90	0.69
1:B:410:PHE:HA	1:B:469:GLY:CA	2.22	0.69
1:A:454:SER:HB2	1:A:457:PHE:HD2	1.58	0.69
1:B:451:ASP:HB3	1:B:454:SER:HB3	1.75	0.69
1:A:395:TYR:HD1	1:A:410:PHE:CE1	2.08	0.68
1:A:429:LYS:HB3	1:A:497:ASP:HB2	1.75	0.68
1:A:396:LEU:CD2	1:A:407:LEU:HD11	2.24	0.68
1:B:479:LEU:HG	1:B:485:ILE:HD11	1.74	0.68
1:B:448:PHE:CD1	1:B:449:LYS:N	2.62	0.67
1:B:470:CYS:HB2	1:B:473:PHE:HB2	1.76	0.67
1:A:354:LEU:CD2	1:A:355:ILE:N	2.58	0.67
1:A:333:ILE:O	1:A:337:ASP:HB2	1.94	0.67
1:A:358:ILE:HB	1:A:490:ILE:CG1	2.25	0.67
1:A:375:SER:HB2	1:A:393:ARG:HE	1.59	0.66
1:B:378:SER:O	1:B:380:PRO:HD3	1.95	0.66
1:B:413:ILE:O	1:B:465:ASN:HB2	1.96	0.66
1:B:390:MET:CE	1:B:496:VAL:HG21	2.26	0.66
1:B:410:PHE:HD2	1:B:469:GLY:HA3	1.61	0.66
1:A:375:SER:HB3	1:A:395:TYR:CD2	2.31	0.66
1:A:477:THR:O	1:A:477:THR:HG23	1.96	0.66
1:A:411:PHE:CE2	1:A:430:VAL:HG21	2.32	0.65
1:B:451:ASP:CG	1:B:452:PRO:HD2	2.17	0.65
1:B:456:SER:CA	1:B:466:ILE:HB	2.25	0.65
1:B:406:HIS:ND1	1:B:475:ALA:HA	2.11	0.65
1:B:386:PHE:HD2	1:B:418:TYR:CE1	2.14	0.65
1:B:424:TRP:HA	1:B:426:PHE:H	1.62	0.65
2:X:261:VAL:HG22	2:X:262:THR:N	2.12	0.65
1:A:350:TYR:CD2	1:A:384:GLY:O	2.49	0.65
1:A:311:ALA:C	1:A:313:ASN:H	1.99	0.65
1:B:500:ASP:O	1:B:501:LEU:HB3	1.97	0.65
1:B:361:TYR:OH	1:B:479:LEU:HD23	1.97	0.65
1:B:456:SER:CB	1:B:466:ILE:HB	2.27	0.64
2:X:252:GLN:N	2:X:252:GLN:NE2	2.40	0.64
1:A:301:GLU:HA	1:A:304:ASP:CG	2.17	0.64
1:A:437:GLN:NE2	1:A:486:LYS:HB2	2.12	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:410:PHE:HB3	1:A:469:GLY:H	1.63	0.63
1:A:431:THR:HB	1:A:495:ILE:HB	1.80	0.63
1:A:389:LYS:HB3	1:A:414:MET:HB2	1.79	0.63
1:A:425:PRO:O	1:A:427:LYS:HG3	1.98	0.63
1:B:438:GLY:O	1:B:440:SER:N	2.32	0.63
2:X:252:GLN:H	2:X:252:GLN:HE21	1.45	0.63
2:Y:255:LEU:HD13	2:Y:256:HIS:N	2.13	0.63
1:B:333:ILE:O	1:B:336:ALA:HB3	1.98	0.63
1:B:358:ILE:HG23	1:B:364:ARG:NH1	2.13	0.63
1:A:447:ALA:O	1:A:448:PHE:HB3	1.97	0.63
1:A:413:ILE:HD12	1:A:456:SER:O	1.99	0.63
1:A:437:GLN:HE21	1:A:486:LYS:N	1.97	0.62
1:B:383:THR:CG2	1:B:388:TYR:HB2	2.28	0.62
1:A:312:ARG:NE	1:A:312:ARG:O	2.32	0.62
1:A:437:GLN:HB2	1:A:486:LYS:HD2	1.81	0.62
1:B:358:ILE:HG23	1:B:364:ARG:HH11	1.63	0.62
1:B:428:GLN:O	1:B:430:VAL:N	2.31	0.62
1:B:303:VAL:CB	1:B:307:ALA:HB3	2.29	0.62
1:B:322:SER:O	1:B:326:GLN:HG3	2.00	0.62
1:A:437:GLN:NE2	1:A:489:THR:O	2.33	0.61
1:B:486:LYS:HD3	1:B:487:ASP:N	2.16	0.61
1:A:307:ALA:O	1:A:310:VAL:HG22	2.01	0.61
1:A:396:LEU:HD23	1:A:407:LEU:HD11	1.83	0.61
1:B:356:TRP:O	1:B:491:PHE:HA	2.00	0.61
1:A:415:ARG:HA	1:A:419:ASP:OD2	2.01	0.60
1:B:449:LYS:HB2	1:B:449:LYS:NZ	2.16	0.60
1:B:409:LEU:HD12	1:B:432:LEU:HB3	1.82	0.60
1:B:431:THR:O	1:B:494:VAL:HG13	2.02	0.60
1:A:385:TYR:N	1:A:385:TYR:CD1	2.69	0.60
1:B:402:GLY:HA3	1:B:472:VAL:HG12	1.84	0.60
1:A:472:VAL:HG23	1:A:472:VAL:O	2.02	0.60
1:B:410:PHE:CD2	1:B:469:GLY:HA3	2.36	0.60
1:A:378:SER:N	1:A:392:ALA:O	2.35	0.60
1:B:450:PRO:HB3	1:B:457:PHE:CD2	2.37	0.60
1:A:441:ARG:HH12	1:A:483:THR:H	1.47	0.60
1:A:409:LEU:HD22	1:A:410:PHE:N	2.17	0.59
2:Y:248:ALA:O	2:Y:249:ALA:HB3	2.03	0.59
1:B:326:GLN:O	1:B:330:VAL:HG23	2.02	0.59
1:A:364:ARG:HG3	1:A:367:GLU:OE1	2.01	0.59
1:A:313:ASN:HA	1:A:316:LEU:HD23	1.84	0.59
2:X:248:ALA:O	2:X:250:PRO:HD3	2.01	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:386:PHE:HB3	1:A:418:TYR:CE2	2.37	0.59
1:A:433:MET:SD	1:A:493:LYS:HE3	2.43	0.59
1:B:309:GLN:HE21	1:B:312:ARG:CG	2.14	0.59
1:B:425:PRO:O	1:B:426:PHE:O	2.19	0.59
1:A:411:PHE:CD2	1:A:430:VAL:HG11	2.37	0.59
1:B:391:CYS:O	1:B:392:ALA:HB2	2.03	0.59
1:B:310:VAL:HG23	1:B:311:ALA:N	2.17	0.59
1:B:429:LYS:HA	1:B:449:LYS:HA	1.85	0.59
1:A:420:ALA:HA	1:A:459:LYS:HE2	1.84	0.59
1:A:488:ASP:O	1:A:489:THR:HG23	2.03	0.59
1:A:376:LEU:HB2	1:A:394:VAL:HG12	1.84	0.58
1:B:454:SER:C	1:B:456:SER:H	2.07	0.58
1:A:436:ASP:OD2	1:A:483:THR:OG1	2.20	0.58
1:A:326:GLN:OE1	1:A:326:GLN:HA	2.03	0.58
1:B:457:PHE:O	1:B:458:LYS:O	2.21	0.58
1:A:496:VAL:O	1:A:498:THR:HG23	2.04	0.58
1:A:486:LYS:C	1:A:488:ASP:N	2.56	0.58
1:B:303:VAL:HB	1:B:307:ALA:HB3	1.86	0.58
1:B:479:LEU:HG	1:B:485:ILE:CD1	2.33	0.58
1:A:486:LYS:C	1:A:488:ASP:H	2.07	0.58
1:A:486:LYS:O	1:A:488:ASP:N	2.37	0.58
1:B:395:TYR:HE1	1:B:410:PHE:CE1	2.21	0.58
1:B:472:VAL:HG23	1:B:472:VAL:O	2.04	0.58
1:B:352:GLY:O	1:B:381:PHE:HE2	1.85	0.58
1:B:456:SER:HA	1:B:466:ILE:CG1	2.34	0.58
1:B:493:LYS:HE2	1:B:495:ILE:CG1	2.32	0.58
1:B:314:THR:O	1:B:317:LEU:N	2.37	0.57
1:B:321:LEU:O	1:B:324:HIS:HB2	2.04	0.57
1:A:411:PHE:CG	1:A:430:VAL:HG11	2.40	0.57
1:A:412:VAL:CG1	1:A:413:ILE:H	2.16	0.57
1:B:314:THR:HG22	1:B:318:GLU:HG3	1.86	0.57
1:B:303:VAL:CA	1:B:307:ALA:HB3	2.34	0.57
1:A:377:TYR:HA	1:A:393:ARG:HA	1.86	0.57
1:A:451:ASP:O	1:A:453:ASN:N	2.37	0.57
1:A:454:SER:HB2	1:A:457:PHE:CD2	2.38	0.57
1:B:355:ILE:CD1	1:B:493:LYS:HB2	2.34	0.57
1:B:340:LEU:O	1:B:344:VAL:HG23	2.04	0.57
1:B:356:TRP:CE3	1:B:492:ILE:HD13	2.40	0.57
1:B:408:SER:HA	1:B:470:CYS:O	2.05	0.57
1:A:412:VAL:CG1	1:A:413:ILE:N	2.68	0.57
1:A:306:SER:HA	1:A:309:GLN:HG3	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:407:LEU:O	1:A:473:PHE:HB3	2.05	0.56
1:A:431:THR:HA	1:A:447:ALA:HA	1.87	0.56
1:B:358:ILE:HB	1:B:490:ILE:CG1	2.35	0.56
1:A:377:TYR:CD2	1:A:393:ARG:HB2	2.40	0.56
1:A:411:PHE:HB2	1:A:432:LEU:HD21	1.88	0.56
1:B:454:SER:O	1:B:456:SER:N	2.38	0.56
1:A:305:LYS:O	1:A:309:GLN:N	2.38	0.56
1:B:312:ARG:CA	1:B:312:ARG:HE	2.10	0.56
1:A:408:SER:CB	1:A:471:PRO:HA	2.32	0.56
1:B:354:LEU:HD13	1:B:354:LEU:O	2.06	0.56
1:A:380:PRO:HG2	1:A:389:LYS:HE2	1.87	0.56
1:B:434:LEU:HD23	1:B:444:LEU:HD12	1.87	0.56
1:A:322:SER:O	1:A:326:GLN:HG2	2.06	0.56
1:B:369:VAL:HG12	1:B:370:MET:N	2.20	0.56
1:B:311:ALA:HA	1:B:314:THR:OG1	2.05	0.55
1:B:480:GLU:CA	1:B:485:ILE:HD12	2.36	0.55
2:X:259:GLN:HB3	2:X:260:PRO:CD	2.33	0.55
1:A:365:LYS:C	1:A:367:GLU:H	2.08	0.55
1:A:378:SER:OG	1:A:392:ALA:HB3	2.07	0.55
1:A:305:LYS:O	1:A:309:GLN:HG3	2.05	0.55
1:A:367:GLU:CB	1:A:373:THR:HB	2.29	0.55
1:B:388:TYR:CE1	1:B:422:LEU:HG	2.41	0.55
1:B:452:PRO:HG2	1:B:453:ASN:OD1	2.07	0.55
1:A:416:GLY:O	1:A:418:TYR:N	2.39	0.55
1:B:486:LYS:HD3	1:B:487:ASP:H	1.71	0.55
2:Y:246:LYS:HD2	2:Y:246:LYS:N	2.21	0.55
1:A:434:LEU:HB2	1:A:473:PHE:HE2	1.71	0.55
1:B:372:LYS:HD3	1:B:373:THR:OG1	2.07	0.55
1:A:437:GLN:NE2	1:A:486:LYS:O	2.40	0.55
1:A:432:LEU:O	1:A:445:GLY:HA3	2.07	0.55
1:B:442:ARG:HH11	1:B:442:ARG:HG2	1.72	0.55
1:B:442:ARG:N	1:B:442:ARG:HD3	2.21	0.54
1:A:358:ILE:HB	1:A:490:ILE:HG12	1.90	0.54
1:B:433:MET:HG3	1:B:435:MET:SD	2.48	0.54
1:A:310:VAL:HA	1:A:313:ASN:OD1	2.07	0.54
1:A:485:ILE:HG22	1:A:485:ILE:O	2.08	0.54
1:A:410:PHE:HA	1:A:469:GLY:HA3	1.89	0.54
1:B:303:VAL:HA	1:B:307:ALA:HB3	1.90	0.54
1:B:314:THR:HA	1:B:317:LEU:HB2	1.89	0.54
1:A:313:ASN:O	1:A:316:LEU:HB2	2.08	0.54
1:B:382:TYR:CE2	1:B:389:LYS:HG3	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:412:VAL:HG11	1:B:464:MET:HB3	1.89	0.54
1:B:456:SER:HA	1:B:466:ILE:CB	2.38	0.54
1:B:410:PHE:CA	1:B:469:GLY:HA3	2.27	0.54
1:A:395:TYR:CD1	1:A:399:ASP:HB3	2.43	0.54
1:A:396:LEU:HD22	1:A:407:LEU:HD11	1.89	0.54
1:B:502:PRO:O	1:B:503:ASP:HB2	2.08	0.53
1:A:352:GLY:O	1:A:353:VAL:CG2	2.55	0.53
1:A:467:ALA:HB3	2:X:253:GLU:OE1	2.08	0.53
1:A:342:PHE:O	1:A:346:GLU:HG3	2.08	0.53
1:B:448:PHE:HB2	2:Y:249:ALA:HA	1.90	0.53
1:A:360:ASP:O	1:A:363:ARG:HB3	2.09	0.53
1:A:367:GLU:HB3	1:A:373:THR:CB	2.30	0.53
1:A:361:TYR:C	1:A:363:ARG:H	2.12	0.53
1:A:364:ARG:CG	1:A:376:LEU:HD11	2.35	0.53
1:B:500:ASP:O	1:B:501:LEU:CB	2.56	0.53
1:B:448:PHE:CG	2:Y:250:PRO:HD3	2.44	0.53
1:B:468:SER:CB	2:Y:252:GLN:HG3	2.36	0.53
1:A:358:ILE:HB	1:A:490:ILE:HG13	1.91	0.52
1:B:356:TRP:CB	1:B:492:ILE:HB	2.36	0.52
2:Y:255:LEU:HD13	2:Y:256:HIS:H	1.75	0.52
1:B:388:TYR:HA	1:B:422:LEU:HD21	1.92	0.52
1:A:437:GLN:CD	1:A:486:LYS:HB2	2.30	0.52
1:B:304:ASP:O	1:B:308:GLY:HA3	2.09	0.52
2:Y:251:VAL:HG23	2:Y:252:GLN:N	2.23	0.52
1:B:381:PHE:CE2	1:B:496:VAL:HB	2.44	0.52
1:A:329:SER:O	1:A:333:ILE:HG13	2.09	0.52
1:A:357:LYS:HB2	1:A:491:PHE:CE2	2.45	0.52
1:B:335:LEU:HA	1:B:338:MET:HB3	1.91	0.52
1:B:343:GLN:HA	1:B:346:GLU:HB2	1.92	0.52
1:A:458:LYS:O	1:A:460:PRO:HD3	2.10	0.52
1:A:424:TRP:CG	1:A:459:LYS:HB2	2.45	0.52
1:B:354:LEU:HB2	1:B:381:PHE:CG	2.45	0.52
1:B:383:THR:OG1	1:B:388:TYR:HB2	2.09	0.52
1:B:358:ILE:HB	1:B:490:ILE:HG13	1.91	0.51
1:A:375:SER:OG	1:A:393:ARG:NH2	2.41	0.51
1:A:424:TRP:CE3	1:A:425:PRO:HA	2.36	0.51
1:B:354:LEU:HB2	1:B:381:PHE:CB	2.40	0.51
1:B:454:SER:C	1:B:456:SER:N	2.64	0.51
1:A:312:ARG:HG2	1:A:312:ARG:HH11	1.76	0.51
2:X:260:PRO:O	2:X:261:VAL:HB	2.10	0.51
1:A:501:LEU:HD22	1:A:502:PRO:HD2	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:375:SER:CB	1:A:393:ARG:NE	2.71	0.51
2:X:261:VAL:CG2	2:X:262:THR:N	2.73	0.51
1:A:473:PHE:CD2	1:A:474:VAL:HG23	2.45	0.51
1:B:451:ASP:OD1	1:B:452:PRO:HD2	2.10	0.51
1:A:424:TRP:NE1	1:A:459:LYS:HG3	2.26	0.51
1:B:449:LYS:HB2	1:B:449:LYS:HZ2	1.74	0.51
2:X:254:THR:OG1	2:X:265:ASP:CA	2.59	0.51
1:A:501:LEU:HD22	1:A:502:PRO:CD	2.41	0.51
1:B:310:VAL:HG23	1:B:311:ALA:H	1.76	0.51
1:A:314:THR:O	1:A:318:GLU:HG3	2.11	0.50
1:A:318:GLU:O	1:A:320:GLN:N	2.45	0.50
1:B:502:PRO:O	1:B:503:ASP:CB	2.59	0.50
1:A:446:ASP:OD2	1:A:447:ALA:N	2.32	0.50
1:B:358:ILE:CG2	1:B:364:ARG:NH1	2.74	0.50
1:B:432:LEU:HD23	1:B:494:VAL:HG13	1.92	0.50
1:A:301:GLU:N	1:A:304:ASP:HB3	2.27	0.50
1:A:310:VAL:O	1:A:313:ASN:HB2	2.12	0.50
1:B:386:PHE:CD2	1:B:418:TYR:CE1	2.98	0.50
1:B:371:GLY:HA2	1:B:374:LEU:HD21	1.94	0.50
1:B:429:LYS:HG2	1:B:449:LYS:HZ2	1.76	0.50
1:A:437:GLN:HE21	1:A:486:LYS:H	1.59	0.50
1:A:447:ALA:O	1:A:448:PHE:CB	2.60	0.49
1:B:342:PHE:O	1:B:345:LEU:N	2.42	0.49
1:B:402:GLY:HA3	1:B:472:VAL:CG1	2.42	0.49
1:A:433:MET:HA	1:A:445:GLY:HA3	1.92	0.49
1:B:337:ASP:O	1:B:340:LEU:HB3	2.11	0.49
1:B:361:TYR:O	1:B:361:TYR:HD1	1.95	0.49
1:B:436:ASP:HB3	1:B:442:ARG:O	2.13	0.49
1:B:350:TYR:CD2	1:B:382:TYR:HD1	2.31	0.49
1:A:361:TYR:OH	1:A:479:LEU:HD21	2.12	0.49
1:A:350:TYR:HD2	1:A:384:GLY:C	2.15	0.49
1:B:406:HIS:CD2	1:B:472:VAL:HG12	2.48	0.49
1:B:350:TYR:N	1:B:350:TYR:CD1	2.80	0.49
1:B:391:CYS:SG	1:B:392:ALA:N	2.85	0.49
1:B:434:LEU:CD2	1:B:444:LEU:HD12	2.42	0.49
1:B:480:GLU:HA	1:B:485:ILE:HD12	1.95	0.49
2:Y:247:THR:HG22	2:Y:248:ALA:N	2.27	0.49
1:B:386:PHE:CD2	1:B:418:TYR:HE1	2.30	0.49
1:A:445:GLY:HA2	1:A:473:PHE:CE1	2.48	0.49
1:A:314:THR:HG22	1:A:318:GLU:OE1	2.13	0.48
1:A:327:MET:HE2	1:A:331:HIS:NE2	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:418:TYR:CD2	1:B:418:TYR:N	2.78	0.48
1:B:435:MET:HG2	1:B:491:PHE:O	2.13	0.48
1:A:342:PHE:HD2	1:A:342:PHE:O	1.97	0.48
1:B:322:SER:CA	1:B:325:ASP:HB2	2.35	0.48
1:B:442:ARG:NH1	1:B:442:ARG:HG2	2.26	0.48
1:B:412:VAL:HG12	1:B:413:ILE:N	2.29	0.48
2:Y:246:LYS:CD	2:Y:246:LYS:N	2.76	0.48
1:A:409:LEU:O	1:A:409:LEU:HD13	2.13	0.48
1:A:433:MET:O	1:A:492:ILE:HG22	2.14	0.48
1:B:330:VAL:HG12	1:B:330:VAL:O	2.13	0.48
1:B:343:GLN:O	1:B:347:THR:HG23	2.14	0.48
1:B:383:THR:HG23	1:B:388:TYR:HB2	1.95	0.48
1:B:428:GLN:O	1:B:430:VAL:HG23	2.13	0.48
1:A:382:TYR:CD1	1:A:382:TYR:N	2.82	0.48
1:B:361:TYR:CE2	1:B:485:ILE:HD11	2.49	0.48
1:A:413:ILE:HD13	1:A:426:PHE:CD2	2.48	0.47
1:B:354:LEU:HB2	1:B:381:PHE:HB3	1.95	0.47
1:B:477:THR:O	1:B:479:LEU:N	2.47	0.47
1:B:323:ARG:HH11	1:B:323:ARG:HG2	1.78	0.47
1:B:358:ILE:CG2	1:B:364:ARG:HH11	2.24	0.47
1:B:360:ASP:HA	1:B:488:ASP:OD2	2.13	0.47
1:A:375:SER:OG	1:A:393:ARG:NE	2.45	0.47
1:A:441:ARG:HH11	1:A:441:ARG:HG3	1.80	0.47
1:B:391:CYS:O	1:B:392:ALA:CB	2.61	0.47
1:A:317:LEU:H	1:A:317:LEU:CD2	2.25	0.47
1:A:361:TYR:CD1	1:A:361:TYR:C	2.88	0.47
1:B:442:ARG:H	1:B:442:ARG:CD	2.22	0.47
1:A:434:LEU:N	1:A:444:LEU:O	2.46	0.47
1:A:483:THR:C	1:A:485:ILE:H	2.18	0.47
1:A:357:LYS:HD2	1:A:491:PHE:CZ	2.50	0.47
1:A:426:PHE:CE1	1:A:428:GLN:HB2	2.44	0.47
1:B:367:GLU:CG	1:B:372:LYS:HD2	2.45	0.47
1:B:477:THR:OG1	1:B:478:VAL:N	2.46	0.47
2:Y:249:ALA:CB	2:Y:250:PRO:CD	2.87	0.47
1:A:312:ARG:HA	1:A:312:ARG:CZ	2.45	0.47
1:A:456:SER:OG	1:A:466:ILE:HG22	2.15	0.47
1:B:381:PHE:HE2	1:B:496:VAL:HB	1.79	0.47
1:A:354:LEU:HB3	1:A:494:VAL:HB	1.96	0.47
1:A:477:THR:O	1:A:477:THR:CG2	2.63	0.47
1:B:361:TYR:CE2	1:B:485:ILE:CD1	2.98	0.47
2:Y:250:PRO:HG2	2:Y:251:VAL:N	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:356:TRP:HZ3	1:A:394:VAL:HB	1.80	0.47
1:A:483:THR:C	1:A:485:ILE:N	2.68	0.47
1:A:356:TRP:CE3	1:A:492:ILE:HD12	2.50	0.46
1:A:366:GLN:O	1:A:372:LYS:HE2	2.15	0.46
1:A:401:MET:HA	1:A:401:MET:CE	2.46	0.46
2:Y:248:ALA:O	2:Y:249:ALA:CB	2.62	0.46
1:B:456:SER:HB3	1:B:466:ILE:HB	1.97	0.46
1:A:311:ALA:C	1:A:313:ASN:N	2.67	0.46
1:A:409:LEU:C	1:A:409:LEU:HD13	2.36	0.46
1:A:409:LEU:HD13	1:A:432:LEU:HD13	1.97	0.46
1:B:312:ARG:O	1:B:316:LEU:HD23	2.16	0.46
1:A:356:TRP:HH2	1:A:394:VAL:HG12	1.80	0.46
1:A:361:TYR:C	1:A:363:ARG:N	2.67	0.46
1:A:385:TYR:HD1	1:A:385:TYR:H	1.62	0.46
1:B:316:LEU:HA	1:B:319:SER:HG	1.81	0.46
2:X:254:THR:O	2:X:255:LEU:HB2	2.15	0.46
1:A:306:SER:O	1:A:309:GLN:HB2	2.16	0.46
1:A:431:THR:HA	1:A:447:ALA:CA	2.45	0.46
1:B:332:ASP:O	1:B:336:ALA:CB	2.56	0.46
1:B:334:ARG:O	1:B:338:MET:HB2	2.16	0.46
1:B:400:GLY:H	2:Y:264:GLU:HG2	1.80	0.46
1:B:422:LEU:HD23	1:B:424:TRP:CH2	2.51	0.46
1:A:436:ASP:OD1	1:A:484:TYR:HA	2.16	0.46
1:B:314:THR:O	1:B:315:GLY:C	2.52	0.46
1:A:317:LEU:N	1:A:317:LEU:HD22	2.28	0.45
1:B:316:LEU:HA	1:B:319:SER:OG	2.16	0.45
1:B:356:TRP:N	1:B:492:ILE:O	2.44	0.45
1:A:389:LYS:O	1:A:414:MET:SD	2.74	0.45
1:B:360:ASP:C	1:B:362:LYS:N	2.67	0.45
1:B:440:SER:C	1:B:441:ARG:HG2	2.36	0.45
2:Y:261:VAL:HG22	2:Y:262:THR:H	1.80	0.45
1:B:309:GLN:NE2	1:B:312:ARG:HG3	2.23	0.45
1:B:375:SER:HB3	1:B:395:TYR:CE2	2.52	0.45
1:B:501:LEU:HD22	1:B:502:PRO:CD	2.38	0.45
1:B:359:ARG:HG3	1:B:489:THR:HG22	1.97	0.45
1:B:452:PRO:HG2	1:B:453:ASN:H	1.81	0.45
1:B:425:PRO:O	1:B:457:PHE:HB3	2.17	0.45
1:B:311:ALA:O	1:B:315:GLY:N	2.42	0.45
1:B:322:SER:O	1:B:325:ASP:HB2	2.17	0.45
1:A:436:ASP:OD1	1:A:484:TYR:N	2.50	0.45
1:A:449:LYS:HE3	2:X:247:THR:HA	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:359:ARG:CB	1:A:489:THR:HG22	2.42	0.45
1:B:352:GLY:O	1:B:381:PHE:CE2	2.69	0.45
1:A:376:LEU:O	1:A:394:VAL:N	2.43	0.45
1:A:399:ASP:CG	1:A:399:ASP:O	2.54	0.45
1:A:456:SER:HG	1:A:466:ILE:HG22	1.82	0.45
1:A:479:LEU:HD12	1:A:484:TYR:HB2	1.99	0.45
1:A:356:TRP:CZ3	1:A:358:ILE:HD11	2.52	0.45
1:B:331:HIS:CD2	1:B:331:HIS:N	2.85	0.45
1:A:386:PHE:HB3	1:A:418:TYR:CG	2.52	0.44
1:B:436:ASP:HB2	1:B:484:TYR:CE1	2.52	0.44
1:A:317:LEU:O	1:A:318:GLU:C	2.55	0.44
1:A:428:GLN:O	1:A:430:VAL:HG23	2.17	0.44
1:B:368:ALA:HA	1:B:373:THR:O	2.16	0.44
1:B:390:MET:HE2	1:B:496:VAL:HG21	1.99	0.44
1:B:501:LEU:C	1:B:501:LEU:HD13	2.38	0.44
1:A:416:GLY:O	1:A:417:GLU:C	2.56	0.44
1:A:376:LEU:O	1:A:393:ARG:HA	2.18	0.44
1:A:380:PRO:HB3	1:A:389:LYS:HG2	1.99	0.44
1:A:496:VAL:O	1:A:498:THR:N	2.50	0.44
1:B:429:LYS:HE2	1:B:449:LYS:NZ	2.32	0.44
1:B:313:ASN:O	1:B:317:LEU:HD23	2.18	0.44
1:B:395:TYR:CD1	1:B:395:TYR:N	2.86	0.44
1:A:436:ASP:HB2	1:A:484:TYR:CE1	2.52	0.44
2:X:254:THR:HB	2:X:255:LEU:H	1.54	0.44
1:A:377:TYR:HA	1:A:392:ALA:O	2.18	0.43
1:A:454:SER:HA	2:X:252:GLN:OE1	2.18	0.43
1:B:376:LEU:N	1:B:394:VAL:O	2.51	0.43
1:B:395:TYR:CE1	1:B:410:PHE:CE1	3.03	0.43
1:A:396:LEU:HA	1:A:407:LEU:CG	2.42	0.43
1:B:363:ARG:O	1:B:367:GLU:HG3	2.19	0.43
1:A:304:ASP:OD1	1:A:305:LYS:HG3	2.17	0.43
1:B:468:SER:HB2	2:Y:252:GLN:CG	2.40	0.43
1:A:475:ALA:O	1:A:478:VAL:N	2.49	0.43
1:B:436:ASP:CB	1:B:442:ARG:O	2.66	0.43
1:B:495:ILE:O	1:B:495:ILE:HG22	2.18	0.43
1:B:501:LEU:O	1:B:502:PRO:C	2.55	0.43
1:A:483:THR:O	1:A:485:ILE:N	2.52	0.43
1:B:361:TYR:O	1:B:361:TYR:CD1	2.72	0.43
1:A:326:GLN:O	1:A:329:SER:HB3	2.19	0.43
1:B:412:VAL:CG1	1:B:464:MET:HB3	2.47	0.43
1:B:425:PRO:O	1:B:457:PHE:CB	2.67	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:480:GLU:HB3	1:B:485:ILE:HD12	2.01	0.43
1:A:327:MET:CE	1:A:331:HIS:NE2	2.81	0.43
1:A:347:THR:O	1:A:379:GLN:NE2	2.51	0.43
1:A:409:LEU:CD1	1:A:432:LEU:HD13	2.49	0.43
1:B:328:LEU:C	1:B:330:VAL:H	2.21	0.42
2:Y:259:GLN:HA	2:Y:260:PRO:HD2	1.85	0.42
1:A:401:MET:HA	1:A:401:MET:HE2	2.00	0.42
1:A:357:LYS:HG3	1:A:491:PHE:CZ	2.55	0.42
1:A:438:GLY:O	1:A:439:SER:O	2.38	0.42
1:B:334:ARG:HD2	1:B:334:ARG:HA	1.76	0.42
1:B:382:TYR:CD2	1:B:382:TYR:N	2.85	0.42
1:A:475:ALA:HB3	1:A:478:VAL:HG23	2.02	0.42
1:B:347:THR:HB	1:B:379:GLN:HG3	2.00	0.42
1:B:431:THR:O	1:B:494:VAL:HA	2.19	0.42
1:B:451:ASP:OD1	2:Y:247:THR:HG21	2.20	0.42
1:A:357:LYS:HG2	1:A:359:ARG:NH1	2.35	0.42
1:A:415:ARG:HB2	1:A:460:PRO:HB3	2.02	0.42
1:B:359:ARG:HG3	1:B:489:THR:CG2	2.49	0.42
1:A:354:LEU:HD22	1:A:355:ILE:N	2.33	0.42
1:A:408:SER:OG	1:A:471:PRO:O	2.32	0.42
1:B:364:ARG:C	1:B:396:LEU:HD12	2.39	0.42
1:B:356:TRP:HB3	1:B:492:ILE:HD12	2.02	0.42
1:A:309:GLN:O	1:A:313:ASN:ND2	2.53	0.41
1:B:430:VAL:HG12	1:B:431:THR:N	2.35	0.41
1:A:365:LYS:C	1:A:367:GLU:N	2.74	0.41
1:A:375:SER:HB2	1:A:393:ARG:NE	2.31	0.41
1:A:350:TYR:CD2	1:A:385:TYR:HA	2.56	0.41
1:B:393:ARG:NH1	2:Y:263:GLN:OE1	2.53	0.41
1:B:354:LEU:HD12	1:B:494:VAL:CG2	2.44	0.41
1:B:360:ASP:O	1:B:364:ARG:HB2	2.20	0.41
1:B:390:MET:HG2	1:B:411:PHE:CZ	2.55	0.41
1:B:465:ASN:HB3	1:B:466:ILE:H	1.69	0.41
2:X:261:VAL:HG22	2:X:262:THR:H	1.85	0.41
1:A:331:HIS:O	1:A:335:LEU:N	2.37	0.41
1:A:433:MET:SD	1:A:495:ILE:HD12	2.61	0.41
1:A:437:GLN:HB2	1:A:486:LYS:CD	2.49	0.41
1:B:358:ILE:HD11	1:B:492:ILE:CD1	2.51	0.41
1:B:429:LYS:H	1:B:429:LYS:HG3	1.72	0.41
1:B:456:SER:HA	1:B:466:ILE:HG13	2.01	0.41
1:A:449:LYS:HA	1:A:450:PRO:HD3	1.87	0.41
1:A:414:MET:HG2	1:A:464:MET:HG3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:383:THR:OG1	1:B:388:TYR:N	2.51	0.41
1:B:463:GLU:HB2	1:B:464:MET:SD	2.61	0.41
2:X:261:VAL:CG2	2:X:262:THR:H	2.34	0.41
1:A:375:SER:CB	1:A:395:TYR:CE2	2.95	0.41
1:B:316:LEU:N	1:B:316:LEU:HD22	2.35	0.41
1:B:359:ARG:O	1:B:364:ARG:NH2	2.54	0.41
1:B:459:LYS:HB3	1:B:459:LYS:HE2	1.93	0.41
1:A:350:TYR:HE2	1:A:385:TYR:HA	1.80	0.40
1:A:446:ASP:CG	1:A:447:ALA:N	2.74	0.40
1:A:451:ASP:HA	1:A:452:PRO:HD2	1.83	0.40
1:A:488:ASP:O	1:A:489:THR:CG2	2.69	0.40
1:B:355:ILE:HD13	1:B:493:LYS:CB	2.48	0.40
2:X:260:PRO:O	2:X:261:VAL:CB	2.67	0.40
1:A:389:LYS:HG2	1:A:389:LYS:O	2.21	0.40
1:A:479:LEU:O	1:A:479:LEU:HD12	2.21	0.40
2:Y:250:PRO:HG2	2:Y:251:VAL:H	1.86	0.40
1:A:425:PRO:O	1:A:426:PHE:C	2.60	0.40
1:A:451:ASP:C	1:A:453:ASN:H	2.25	0.40
1:A:363:ARG:O	1:A:367:GLU:HG3	2.22	0.40
1:A:377:TYR:OH	1:A:393:ARG:CZ	2.70	0.40
1:B:448:PHE:CD2	2:Y:250:PRO:HG3	2.56	0.40
1:A:340:LEU:O	1:A:344:VAL:HG23	2.22	0.40
1:A:359:ARG:HA	1:A:489:THR:HG22	2.04	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	203/228 (89%)	144 (71%)	36 (18%)	23 (11%)	0	6
1	B	203/228 (89%)	139 (68%)	38 (19%)	26 (13%)	0	5

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	X	19/21 (90%)	9 (47%)	4 (21%)	6 (32%)	0	0
2	Y	19/21 (90%)	7 (37%)	8 (42%)	4 (21%)	0	1
All	All	444/498 (89%)	299 (67%)	86 (19%)	59 (13%)	0	4

All (59) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	301	GLU
1	A	318	GLU
1	A	319	SER
1	A	371	GLY
1	A	417	GLU
1	A	439	SER
1	A	441	ARG
1	A	448	PHE
1	A	460	PRO
1	A	497	ASP
1	A	499	SER
2	X	261	VAL
1	B	362	LYS
1	B	392	ALA
1	B	426	PHE
1	B	429	LYS
1	B	439	SER
1	B	458	LYS
1	B	478	VAL
1	B	501	LEU
1	B	502	PRO
1	B	503	ASP
2	Y	249	ALA
2	Y	250	PRO
1	A	374	LEU
1	A	452	PRO
1	A	463	GLU
1	A	487	ASP
2	X	255	LEU
2	X	256	HIS
2	X	258	SER
2	X	263	GLN
1	B	391	CYS
1	B	455	SER

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Mol	Chain	Res	Type
1	B	484	TYR
2	Y	255	LEU
1	A	372	LYS
1	A	390	MET
1	A	402	GLY
1	A	418	TYR
1	B	329	SER
1	B	360	ASP
1	B	380	PRO
1	B	402	GLY
1	B	415	ARG
1	B	452	PRO
1	B	454	SER
1	B	460	PRO
1	B	477	THR
1	A	351	ASN
1	A	438	GLY
1	B	369	VAL
2	Y	258	SER
1	A	366	GLN
1	A	401	MET
1	B	303	VAL
1	B	370	MET
1	B	379	GLN
2	X	250	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	179/201 (89%)	151 (84%)	28 (16%)	3	18
1	B	179/201 (89%)	157 (88%)	22 (12%)	5	27
2	X	17/17 (100%)	12 (71%)	5 (29%)	0	3
2	Y	17/17 (100%)	14 (82%)	3 (18%)	2	12
All	All	392/436 (90%)	334 (85%)	58 (15%)	3	20

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	304	ASP
1	A	310	VAL
1	A	312	ARG
1	A	317	LEU
1	A	325	ASP
1	A	340	LEU
1	A	342	PHE
1	A	343	GLN
1	A	347	THR
1	A	351	ASN
1	A	354	LEU
1	A	364	ARG
1	A	365	LYS
1	A	382	TYR
1	A	385	TYR
1	A	399	ASP
1	A	401	MET
1	A	409	LEU
1	A	418	TYR
1	A	423	PRO
1	A	426	PHE
1	A	443	HIS
1	A	465	ASN
1	A	477	THR
1	A	479	LEU
1	A	481	ASN
1	A	492	ILE
1	A	497	ASP
2	X	250	PRO
2	X	251	VAL
2	X	252	GLN
2	X	253	GLU
2	X	256	HIS
1	B	312	ARG
1	B	321	LEU
1	B	327	MET
1	B	342	PHE
1	B	350	TYR
1	B	351	ASN
1	B	354	LEU
1	B	372	LYS
1	B	379	GLN

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Mol	Chain	Res	Type
1	B	390	MET
1	B	394	VAL
1	B	397	ASN
1	B	401	MET
1	B	409	LEU
1	B	413	ILE
1	B	419	ASP
1	B	441	ARG
1	B	442	ARG
1	B	453	ASN
1	B	465	ASN
1	B	476	GLN
1	B	480	GLU
2	Y	250	PRO
2	Y	251	VAL
2	Y	255	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	309	GLN
1	A	313	ASN
1	A	351	ASN
1	A	437	GLN
1	A	465	ASN
2	X	252	GLN
2	X	256	HIS
1	B	309	GLN
1	B	324	HIS
1	B	331	HIS
1	B	397	ASN
1	B	428	GLN
1	B	465	ASN
1	B	476	GLN

### 5.3.3 RNA ⓘ

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](#)

There are no ligands in this entry.

## 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	205/228 (89%)	0.26	5 (2%) 59 50	15, 33, 67, 76	0
1	B	205/228 (89%)	0.27	5 (2%) 59 50	15, 33, 67, 76	0
2	X	21/21 (100%)	0.87	3 (14%) 3 4	13, 15, 17, 48	0
2	Y	21/21 (100%)	0.91	4 (19%) 1 2	13, 15, 17, 48	0
All	All	452/498 (90%)	0.32	17 (3%) 41 35	13, 31, 67, 76	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	300	LEU	6.5
2	Y	266	GLY	4.9
2	Y	262	THR	3.3
1	B	300	LEU	2.9
1	B	485	ILE	2.9
1	A	310	VAL	2.8
1	B	306	SER	2.8
1	A	306	SER	2.5
1	A	503	ASP	2.5
2	Y	254	THR	2.5
2	X	247	THR	2.4
2	Y	265	ASP	2.3
2	X	262	THR	2.3
2	X	248	ALA	2.2
1	A	309	GLN	2.1
1	B	304	ASP	2.0
1	B	428	GLN	2.0

### 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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](#)

There are no ligands in this entry.

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

There are no such residues in this entry.