



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:25 PM GMT

PDB ID : 4LKO  
Title : Crystal structure of human DPP-IV in complex with BMS-744891  
Authors : Klei, H.E.  
Deposited on : 2013-07-08  
Resolution : 2.43 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

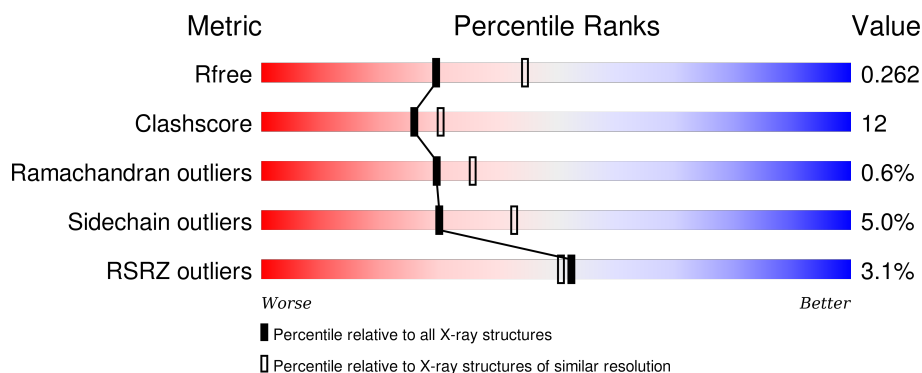
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.43 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	1003 (2.46-2.42)
Clashscore	102246	1071 (2.46-2.42)
Ramachandran outliers	100387	1065 (2.46-2.42)
Sidechain outliers	100360	1065 (2.46-2.42)
RSRZ outliers	91569	1005 (2.46-2.42)

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	728	<div> <div>3%</div> <div>75%</div> <div>22%</div> <div>.</div> </div>
1	B	728	<div> <div>4%</div> <div>72%</div> <div>25%</div> <div>.</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
2	1WH	B	801	-	-	-	X

## 2 Entry composition [i](#)

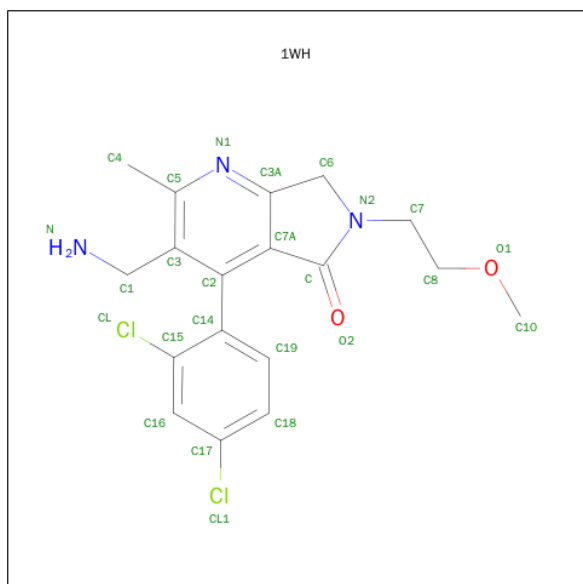
There are 3 unique types of molecules in this entry. The entry contains 12074 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Dipeptidyl peptidase 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	728	Total	C	N	O	S	0	0	0
			5963	3827	982	1128	26			
1	B	728	Total	C	N	O	S	0	0	0
			5963	3827	982	1128	26			

- Molecule 2 is 3-(AMINOMETHYL)-4-(2,4-DICHLOROPHENYL)-6-(2-METHOXYETHYL)-2-METHYL-6,7-DIHYDRO-5H-PYRROLO[3,4-B]PYRIDIN-5-ONE (three-letter code: 1WH) (formula: C<sub>18</sub>H<sub>19</sub>Cl<sub>2</sub>N<sub>3</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Cl	N	O	0	0
			25	18	2	3	2		
2	B	1	Total	C	Cl	N	O	0	0
			25	18	2	3	2		

- Molecule 3 is water.

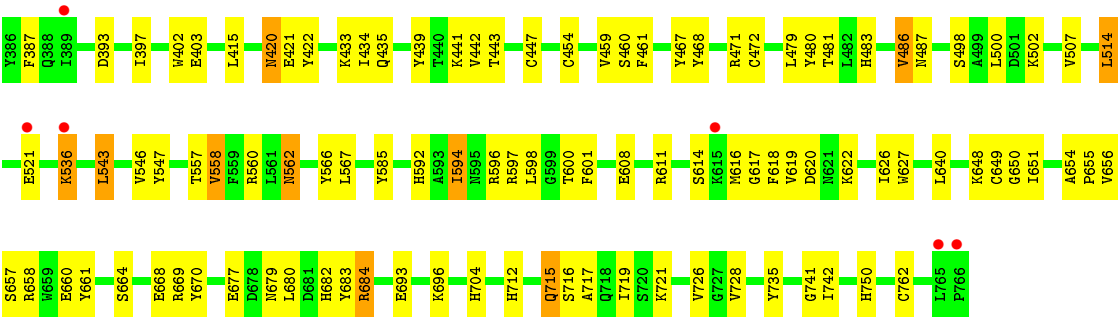
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	63	Total 63	O 63	0	0
3	B	35	Total 35	O 35	0	0

### 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: Dipeptidyl peptidase 4





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	65.90 Å 68.30 Å 421.50 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.43 – 2.43 47.42 – 2.43	Depositor EDS
% Data completeness (in resolution range)	96.4 (47.43-2.43) 96.5 (47.42-2.43)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.63 (at 2.42 Å)	Xtriage
Refinement program	CNX 2002	Depositor
R, $R_{free}$	0.226 , 0.263 0.226 , 0.262	Depositor DCC
$R_{free}$ test set	4996 reflections (7.66%)	DCC
Wilson B-factor (Å <sup>2</sup> )	50.5	Xtriage
Anisotropy	0.543	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 30.0	EDS
Estimated twinning fraction	0.064 for k,h,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 70190 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	12074	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.07% 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 [i](#)

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

Bond lengths and bond angles in the following residue types are not validated in this section: 1WH

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	0/6135	0.67	0/8344
1	B	0.36	0/6135	0.66	1/8344 (0.0%)
All	All	0.38	0/12270	0.66	1/16688 (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	B	300	LEU	N-CA-C	-5.00	97.49	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	547	TYR	Sidechain

### 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	5963	0	5695	135	0
1	B	5963	0	5695	157	0
2	A	25	0	19	0	0
2	B	25	0	19	0	0
3	A	63	0	0	1	0
3	B	35	0	0	0	0
All	All	12074	0	11428	285	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 12.

All (285) 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:508:GLN:HE21	1:A:533:HIS:CE1	1.76	1.04
1:B:600:THR:HG23	1:B:601:PHE:H	1.22	0.99
1:B:51:ASN:HD22	1:B:54:ARG:HG2	1.32	0.95
1:B:177:GLU:HB2	1:B:180:LEU:HD23	1.49	0.95
1:A:508:GLN:HE21	1:A:533:HIS:HE1	0.99	0.93
1:A:385:CYS:HG	1:A:394:CYS:HG	1.21	0.89
1:B:649:CYS:HG	1:B:762:CYS:HG	1.21	0.88
1:A:403:GLU:H	1:A:420:ASN:HD21	1.24	0.85
1:B:600:THR:HG23	1:B:601:PHE:N	1.91	0.83
1:B:77:LEU:HD23	1:B:88:VAL:HA	1.61	0.82
1:A:39:SER:HB2	1:A:508:GLN:HG3	1.59	0.82
1:A:89:PHE:HE2	1:A:107:ILE:HD13	1.45	0.81
1:A:693:GLU:O	1:A:696:LYS:HG3	1.81	0.81
1:A:328:CYS:HG	1:A:339:CYS:HG	1.16	0.80
1:B:403:GLU:H	1:B:420:ASN:HD21	1.29	0.80
1:A:508:GLN:NE2	1:A:533:HIS:HE1	1.80	0.79
1:B:600:THR:CG2	1:B:601:PHE:H	1.96	0.79
1:B:89:PHE:HE2	1:B:107:ILE:HD13	1.47	0.78
1:A:649:CYS:HG	1:A:762:CYS:HG	0.77	0.77
1:A:340:LEU:HB3	1:A:343:ARG:HD3	1.66	0.77
1:B:471:ARG:HG3	1:B:480:TYR:CE2	2.20	0.76
1:A:377:ASN:C	1:A:377:ASN:HD22	1.88	0.76
1:B:221:THR:O	1:B:273:THR:HG22	1.85	0.76
1:B:536:LYS:HD3	1:B:536:LYS:H	1.49	0.76
1:B:320:GLN:OE1	1:B:669:ARG:HD3	1.86	0.76
1:A:657:SER:H	1:A:715:GLN:NE2	1.84	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:142:LEU:HD12	1:A:142:LEU:H	1.52	0.75
1:B:726:VAL:HG13	1:B:728:VAL:HG23	1.69	0.74
1:A:726:VAL:HG12	1:A:728:VAL:HG23	1.69	0.74
1:B:735:TYR:OH	1:B:750:HIS:HD2	1.71	0.73
1:B:597:ARG:O	1:B:600:THR:HG22	1.87	0.73
1:A:499:ALA:HA	1:A:502:LYS:HE3	1.70	0.72
1:B:236:ILE:HD13	1:B:237:GLU:N	2.04	0.72
1:A:236:ILE:HG13	1:A:712:HIS:CE1	2.26	0.71
1:B:358:ARG:HH21	1:B:358:ARG:HB3	1.55	0.70
1:B:219:ASN:HB2	1:B:308:GLN:OE1	1.91	0.70
1:B:358:ARG:NH2	1:B:358:ARG:HB3	2.07	0.70
1:B:657:SER:H	1:B:715:GLN:NE2	1.89	0.70
1:A:237:GLU:OE2	1:A:253:ARG:HD3	1.92	0.69
1:B:236:ILE:HG13	1:B:712:HIS:CE1	2.27	0.69
1:B:217:SER:OG	1:B:222:PHE:HB2	1.92	0.69
1:B:89:PHE:CE2	1:B:107:ILE:HD13	2.27	0.68
1:B:175:LYS:HG3	1:B:182:SER:HB3	1.75	0.68
1:A:500:LEU:HD22	1:A:504:LEU:HG	1.76	0.67
1:B:481:THR:OG1	1:B:483:HIS:HE1	1.77	0.67
1:A:89:PHE:CE2	1:A:107:ILE:HD13	2.29	0.67
1:B:139:LYS:C	1:B:140:ARG:HD2	2.15	0.67
1:A:508:GLN:NE2	1:A:533:HIS:CE1	2.58	0.66
1:B:377:ASN:HD22	1:B:377:ASN:C	1.97	0.66
1:B:640:LEU:HD11	1:B:650:GLY:HA3	1.78	0.66
1:A:237:GLU:HG2	1:A:253:ARG:HG2	1.80	0.64
1:A:696:LYS:HD2	1:A:697:GLN:HG3	1.79	0.64
1:B:196:ASN:OD1	1:B:227:GLN:HG3	1.98	0.64
1:A:343:ARG:N	1:A:343:ARG:HD2	2.13	0.64
1:A:481:THR:OG1	1:A:483:HIS:HE1	1.81	0.63
1:B:78:VAL:HG23	1:B:89:PHE:HB2	1.80	0.63
1:B:677:GLU:H	1:B:677:GLU:CD	2.01	0.63
1:B:558:VAL:HG22	1:B:560:ARG:NH1	2.13	0.63
1:A:735:TYR:OH	1:A:750:HIS:HD2	1.81	0.62
1:B:51:ASN:ND2	1:B:54:ARG:HG2	2.12	0.62
1:B:60:LEU:H	1:B:60:LEU:HD22	1.64	0.62
1:A:343:ARG:HD2	1:A:343:ARG:H	1.63	0.62
1:B:102:ILE:HD13	1:B:116:LEU:HD22	1.81	0.62
1:B:111:GLY:O	1:B:137:LEU:HD12	2.00	0.61
1:B:306:ALA:HB3	1:B:310:ARG:HG2	1.81	0.61
1:A:377:ASN:ND2	1:A:379:GLU:H	1.99	0.60
1:A:142:LEU:N	1:A:142:LEU:HD12	2.15	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:143:ILE:HG13	1:B:143:ILE:O	2.01	0.59
1:A:139:LYS:O	1:A:140:ARG:HB2	2.01	0.59
1:B:177:GLU:CB	1:B:180:LEU:HD23	2.30	0.59
1:A:160:VAL:HG12	1:A:161:GLY:N	2.18	0.59
1:A:510:PRO:HD3	1:A:569:SER:HB2	1.85	0.58
1:B:514:LEU:HD12	1:B:557:THR:HG22	1.85	0.58
1:A:193:ILE:HG22	1:A:194:ILE:HG12	1.85	0.57
1:B:269:PHE:CE1	1:B:286:GLN:HB2	2.39	0.57
1:B:91:GLU:CD	1:B:91:GLU:H	2.07	0.57
1:B:46:THR:CG2	1:B:50:LYS:HD3	2.35	0.57
1:A:405:ILE:HD13	1:A:419:SER:HA	1.84	0.57
1:A:289:ALA:HB3	1:A:294:LEU:CD1	2.35	0.57
1:B:403:GLU:H	1:B:420:ASN:ND2	2.00	0.57
1:B:614:SER:HA	1:B:619:VAL:CG2	2.34	0.57
1:B:680:LEU:C	1:B:680:LEU:HD13	2.26	0.56
1:B:614:SER:HA	1:B:619:VAL:HG21	1.87	0.56
1:B:454:CYS:CB	1:B:472:CYS:SG	2.92	0.56
1:A:377:ASN:ND2	1:A:377:ASN:C	2.54	0.56
1:A:454:CYS:CB	1:A:472:CYS:SG	2.93	0.56
1:A:242:SER:OG	1:A:243:ASP:N	2.38	0.56
1:B:459:VAL:HG22	1:B:460:SER:N	2.20	0.56
1:B:454:CYS:SG	1:B:472:CYS:SG	3.04	0.56
1:A:341:VAL:HG12	1:A:341:VAL:O	2.06	0.56
1:B:63:ILE:HD11	1:B:109:PRO:O	2.05	0.56
1:A:403:GLU:H	1:A:420:ASN:ND2	2.00	0.56
1:A:236:ILE:HD13	1:A:237:GLU:N	2.20	0.55
1:B:486:VAL:HG12	1:B:487:ASN:OD1	2.05	0.55
1:B:704:HIS:ND1	1:B:716:SER:HB2	2.21	0.55
1:A:72:GLN:O	1:A:73:GLU:HB2	2.07	0.55
1:A:454:CYS:SG	1:A:472:CYS:SG	3.03	0.55
1:B:377:ASN:HD21	1:B:381:TYR:H	1.53	0.55
1:A:736:THR:HG21	1:B:717:ALA:O	2.07	0.55
1:B:373:LYS:HD3	1:B:375:ILE:HD11	1.88	0.54
1:B:657:SER:H	1:B:715:GLN:HE21	1.55	0.54
1:A:224:ALA:HB1	1:A:268:PHE:CZ	2.43	0.54
1:A:385:CYS:HB3	1:A:387:PHE:CE1	2.41	0.54
1:B:377:ASN:C	1:B:377:ASN:ND2	2.61	0.54
1:B:454:CYS:CB	1:B:472:CYS:HG	2.20	0.54
1:B:45:LEU:HG	1:B:49:LEU:HD22	1.89	0.54
1:A:528:MET:HE3	1:A:530:LEU:HD21	1.90	0.54
1:B:454:CYS:HB3	1:B:472:CYS:SG	2.48	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:514:LEU:HD12	1:A:557:THR:HG22	1.91	0.54
1:B:154:TRP:NE1	1:B:156:THR:OG1	2.41	0.54
1:A:736:THR:CG2	1:B:721:LYS:HB2	2.39	0.53
1:A:657:SER:H	1:A:715:GLN:HE21	1.55	0.53
1:B:693:GLU:O	1:B:696:LYS:HG2	2.08	0.53
1:B:236:ILE:HD13	1:B:237:GLU:H	1.74	0.53
1:A:242:SER:HB3	1:A:246:LEU:HD12	1.90	0.53
1:B:377:ASN:ND2	1:B:381:TYR:H	2.06	0.53
1:A:271:VAL:HG22	1:A:284:SER:HA	1.90	0.53
1:B:415:LEU:HD23	1:B:415:LEU:C	2.29	0.52
1:A:77:LEU:HD23	1:A:88:VAL:HA	1.92	0.52
1:A:48:TYR:CD2	1:A:49:LEU:HD12	2.45	0.52
1:A:451:PRO:HG2	1:A:452:GLU:OE2	2.09	0.52
1:A:454:CYS:HB3	1:A:472:CYS:SG	2.49	0.52
1:A:674:PRO:O	1:A:680:LEU:HD13	2.10	0.51
1:B:600:THR:CG2	1:B:601:PHE:N	2.61	0.51
1:B:82:GLU:HB2	1:B:467:TYR:OH	2.11	0.51
1:B:459:VAL:HG22	1:B:460:SER:H	1.76	0.51
1:A:528:MET:CE	1:A:530:LEU:HD21	2.41	0.51
1:B:150:ASN:O	1:B:151:ASN:HB2	2.11	0.51
1:B:144:THR:O	1:B:144:THR:HG22	2.11	0.51
1:A:369:ASN:O	1:A:389:ILE:HG12	2.10	0.51
1:B:403:GLU:OE1	1:B:585:TYR:HA	2.10	0.50
1:B:726:VAL:CG1	1:B:728:VAL:HG23	2.39	0.50
1:A:420:ASN:C	1:A:420:ASN:HD22	2.15	0.50
1:A:684:ARG:HG3	1:A:684:ARG:HH11	1.76	0.50
1:B:197:GLY:HA2	1:B:214:LEU:HD13	1.94	0.50
1:A:543:LEU:HD12	1:A:567:LEU:HD13	1.94	0.50
1:A:45:LEU:O	1:A:49:LEU:HD13	2.12	0.49
1:B:562:ASN:HD22	1:B:562:ASN:C	2.15	0.49
1:A:446:SER:HB2	1:A:457:TYR:CE2	2.47	0.49
1:B:139:LYS:HD3	1:B:141:GLN:NE2	2.27	0.49
1:A:415:LEU:C	1:A:415:LEU:HD23	2.33	0.49
1:A:289:ALA:HB3	1:A:294:LEU:HD11	1.94	0.49
1:B:290:PRO:HG3	1:B:326:ASP:OD2	2.13	0.49
1:B:422:TYR:CD1	1:B:447:CYS:SG	3.06	0.48
1:B:314:GLN:HG2	1:B:325:MET:HG3	1.95	0.48
1:B:69:LEU:CD2	1:B:78:VAL:HG22	2.44	0.48
1:B:546:VAL:HG22	1:B:547:TYR:N	2.28	0.48
1:B:648:LYS:HE3	1:B:762:CYS:SG	2.53	0.48
1:B:129:THR:HG23	1:B:151:ASN:HA	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:109:PRO:HG2	1:A:158:SER:O	2.14	0.48
1:B:741:GLY:O	1:B:742:ILE:C	2.52	0.48
1:A:750:HIS:HE1	1:B:728:VAL:O	1.97	0.48
1:A:219:ASN:N	1:A:308:GLN:OE1	2.47	0.47
1:B:146:GLU:O	1:B:175:LYS:NZ	2.41	0.47
1:B:461:PHE:CD1	1:B:468:TYR:HB3	2.49	0.47
1:A:163:LYS:HZ3	1:A:273:THR:HG22	1.79	0.47
1:A:630:SER:OG	1:A:631:TYR:N	2.47	0.47
1:A:458:SER:OG	1:A:471:ARG:HD3	2.15	0.47
1:A:169:ASN:O	1:A:170:ASN:HB2	2.15	0.47
1:A:403:GLU:OE1	1:A:585:TYR:HA	2.15	0.47
1:B:536:LYS:CD	1:B:536:LYS:H	2.22	0.47
1:A:519:LEU:HA	1:A:519:LEU:HD23	1.71	0.47
1:A:530:LEU:HA	1:A:531:PRO:HD3	1.82	0.47
1:B:521:GLU:HG2	1:B:521:GLU:O	2.15	0.47
1:B:285:ILE:N	1:B:285:ILE:HD12	2.29	0.47
1:B:75:ASN:HD21	1:B:92:ASN:ND2	2.13	0.47
1:A:630:SER:HB2	1:A:740:HIS:NE2	2.29	0.46
1:A:146:GLU:HG3	1:A:181:PRO:N	2.30	0.46
1:A:60:LEU:HD13	3:A:960:HOH:O	2.16	0.46
1:B:60:LEU:H	1:B:60:LEU:CD2	2.26	0.46
1:B:140:ARG:HD2	1:B:140:ARG:N	2.29	0.46
1:A:459:VAL:HG22	1:A:460:SER:N	2.31	0.46
1:A:696:LYS:CD	1:A:697:GLN:HG3	2.46	0.46
1:A:377:ASN:ND2	1:A:379:GLU:N	2.64	0.46
1:A:197:GLY:C	1:A:213:ALA:HB3	2.36	0.46
1:B:305:TRP:CZ3	1:B:311:ILE:HG12	2.50	0.46
1:B:608:GLU:OE1	1:B:611:ARG:HD2	2.15	0.46
1:A:372:TYR:HA	1:A:385:CYS:O	2.16	0.46
1:A:160:VAL:CG1	1:A:161:GLY:N	2.79	0.46
1:A:48:TYR:CE1	1:A:562:ASN:HA	2.50	0.46
1:B:110:ASP:O	1:B:112:GLN:N	2.49	0.46
1:B:498:SER:O	1:B:502:LYS:HG3	2.15	0.46
1:B:627:TRP:HB2	1:B:651:ILE:HB	1.99	0.45
1:B:597:ARG:O	1:B:600:THR:CG2	2.63	0.45
1:A:236:ILE:HG13	1:A:712:HIS:ND1	2.30	0.45
1:A:90:LEU:HD23	1:A:90:LEU:HA	1.70	0.45
1:B:263:ASN:HA	1:B:263:ASN:HD22	1.60	0.45
1:B:163:LYS:HZ3	1:B:273:THR:HG23	1.82	0.45
1:B:94:THR:O	1:B:95:PHE:HB2	2.16	0.45
1:A:736:THR:HG23	1:B:721:LYS:HB2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:375:ILE:HG22	1:A:376:SER:O	2.17	0.45
1:A:159:PRO:HD3	1:A:216:TRP:CB	2.47	0.45
1:A:461:PHE:CD1	1:A:468:TYR:HB3	2.52	0.44
1:B:658:ARG:HB3	1:B:661:TYR:CD2	2.53	0.44
1:B:351:THR:HG22	1:B:592:HIS:HB3	1.99	0.44
1:B:102:ILE:HD11	1:B:116:LEU:HD13	1.99	0.44
1:A:60:LEU:HD13	1:A:60:LEU:H	1.83	0.44
1:A:95:PHE:HB3	1:A:98:PHE:HB2	1.99	0.44
1:B:558:VAL:CG2	1:B:560:ARG:CZ	2.94	0.44
1:B:288:THR:HG22	1:B:289:ALA:O	2.18	0.44
1:B:123:GLN:HG2	1:B:124:TRP:N	2.32	0.44
1:B:434:ILE:HG23	1:B:442:VAL:HG22	1.98	0.44
1:A:482:LEU:HD23	1:A:483:HIS:H	1.81	0.44
1:A:280:THR:HG22	1:A:281:ASN:N	2.33	0.44
1:A:513:LYS:O	1:A:527:GLN:HA	2.18	0.44
1:B:208:PHE:HZ	1:B:300:LEU:CD1	2.31	0.44
1:B:402:TRP:CD2	1:B:421:GLU:HB2	2.53	0.44
1:B:137:LEU:O	1:B:139:LYS:O	2.36	0.44
1:A:56:LYS:O	1:A:57:LEU:HD23	2.18	0.44
1:A:116:LEU:O	1:A:132:TYR:HA	2.18	0.44
1:B:594:ILE:HG23	1:B:594:ILE:O	2.17	0.44
1:B:46:THR:HG23	1:B:50:LYS:HD3	1.99	0.44
1:B:331:ASP:O	1:B:335:GLY:N	2.50	0.44
1:B:664:SER:HB2	1:B:668:GLU:OE2	2.18	0.43
1:A:127:SER:O	1:A:128:TYR:HB3	2.18	0.43
1:B:657:SER:HB3	1:B:719:ILE:HD11	2.01	0.43
1:A:594:ILE:CD1	1:A:601:PHE:HB2	2.48	0.43
1:A:594:ILE:O	1:A:594:ILE:HG23	2.17	0.43
1:A:305:TRP:CH2	1:A:311:ILE:HD11	2.53	0.43
1:B:328:CYS:SG	1:B:339:CYS:SG	3.04	0.43
1:A:343:ARG:CD	1:A:343:ARG:H	2.24	0.43
1:B:680:LEU:CD2	1:B:684:ARG:HD3	2.48	0.43
1:B:596:ARG:HA	1:B:670:TYR:O	2.19	0.43
1:B:598:LEU:O	1:B:682:HIS:HE1	2.01	0.43
1:B:616:MET:HB3	1:B:618:PHE:CE2	2.54	0.43
1:B:435:GLN:HE22	1:B:441:LYS:HD2	1.83	0.43
1:B:660:GLU:HG3	1:B:683:TYR:CD2	2.54	0.43
1:B:309:GLU:HB3	1:B:330:TYR:HB3	2.01	0.43
1:A:627:TRP:HB2	1:A:651:ILE:HB	2.01	0.43
1:A:668:GLU:HG2	1:A:673:LEU:HD23	2.01	0.42
1:A:208:PHE:HZ	1:A:300:LEU:HD13	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:60:LEU:O	1:B:60:LEU:HD23	2.19	0.42
1:B:742:ILE:HG22	1:B:742:ILE:O	2.18	0.42
1:B:626:ILE:O	1:B:650:GLY:HA2	2.19	0.42
1:B:543:LEU:HD12	1:B:567:LEU:HD13	2.01	0.42
1:A:736:THR:HG21	1:B:721:LYS:HB2	2.00	0.42
1:A:60:LEU:C	1:A:60:LEU:HD22	2.39	0.42
1:B:611:ARG:HG2	1:B:611:ARG:HH11	1.83	0.42
1:A:397:ILE:HG13	1:A:398:THR:HG23	2.00	0.42
1:B:46:THR:HG22	1:B:50:LYS:HD3	2.00	0.42
1:A:71:LYS:HA	1:A:75:ASN:O	2.19	0.42
1:A:588:ASP:HB3	1:A:592:HIS:CD2	2.54	0.42
1:B:41:LYS:HE3	1:B:53:TYR:OH	2.19	0.42
1:A:764:SER:O	1:A:766:PRO:HD3	2.19	0.42
1:B:93:SER:O	1:B:96:ASP:HB2	2.19	0.42
1:A:234:PRO:HB2	1:B:248:TYR:CZ	2.54	0.42
1:A:236:ILE:C	1:A:236:ILE:HD13	2.39	0.42
1:B:558:VAL:HG22	1:B:560:ARG:CZ	2.49	0.42
1:B:385:CYS:HB3	1:B:387:PHE:CE1	2.54	0.42
1:A:69:LEU:CD1	1:A:107:ILE:HD12	2.50	0.42
1:A:142:LEU:H	1:A:142:LEU:CD1	2.27	0.42
1:A:528:MET:HE3	1:A:528:MET:HB2	1.93	0.42
1:A:320:GLN:OE1	1:A:669:ARG:HD3	2.20	0.42
1:B:114:ILE:HG23	1:B:135:TYR:HB3	2.02	0.42
1:A:122:LYS:HG3	1:A:123:GLN:N	2.33	0.42
1:B:656:VAL:HG13	1:B:715:GLN:HE22	1.85	0.41
1:A:664:SER:HB2	1:A:668:GLU:OE2	2.20	0.41
1:B:654:ALA:N	1:B:655:PRO:CD	2.83	0.41
1:A:464:GLU:O	1:A:464:GLU:HG2	2.20	0.41
1:A:728:VAL:O	1:B:750:HIS:HE1	2.03	0.41
1:A:168:TRP:O	1:A:169:ASN:HB2	2.21	0.41
1:B:677:GLU:CD	1:B:677:GLU:N	2.72	0.41
1:A:60:LEU:O	1:A:60:LEU:HD22	2.20	0.41
1:A:327:ILE:HG13	1:A:343:ARG:HB2	2.03	0.41
1:B:536:LYS:HD3	1:B:536:LYS:N	2.27	0.41
1:B:433:LYS:HG2	1:B:443:THR:HG23	2.03	0.41
1:A:677:GLU:HG3	1:A:678:ASP:N	2.36	0.41
1:B:500:LEU:O	1:B:500:LEU:HD13	2.20	0.41
1:B:329:ASP:OD2	1:B:343:ARG:NH1	2.53	0.41
1:B:137:LEU:HD23	1:B:137:LEU:HA	1.86	0.40
1:A:470:LEU:HD23	1:A:470:LEU:HA	1.99	0.40
1:A:330:TYR:HB2	1:A:337:TRP:CH2	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:626:ILE:O	1:A:650:GLY:HA2	2.21	0.40
1:B:620:ASP:OD1	1:B:622:LYS:HE2	2.21	0.40
1:B:594:ILE:CD1	1:B:601:PHE:HB2	2.52	0.40
1:B:277:SER:HB3	1:B:280:THR:HB	2.02	0.40
1:A:206:GLU:OE2	1:A:663:ASP:OD2	2.39	0.40
1:B:246:LEU:HA	1:B:246:LEU:HD23	1.92	0.40
1:A:544:LEU:HD23	1:A:544:LEU:HA	1.73	0.40
1:A:144:THR:HG22	1:A:147:ARG:HH21	1.86	0.40
1:A:481:THR:OG1	1:A:483:HIS:CE1	2.69	0.40
1:B:546:VAL:CG2	1:B:547:TYR:N	2.84	0.40
1:A:221:THR:O	1:A:273:THR:HB	2.21	0.40
1:B:596:ARG:N	1:B:670:TYR:O	2.51	0.40
1:B:397:ILE:HG13	1:B:439:TYR:CE1	2.56	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	726/728 (100%)	675 (93%)	47 (6%)	4 (1%)	30	36
1	B	726/728 (100%)	682 (94%)	39 (5%)	5 (1%)	26	32
All	All	1452/1456 (100%)	1357 (94%)	86 (6%)	9 (1%)	30	36

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	389	ILE
1	B	111	GLY
1	B	320	GLN
1	A	320	GLN
1	A	617	GLY

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Mol	Chain	Res	Type
1	B	617	GLY
1	B	393	ASP
1	A	486	VAL
1	B	486	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	653/653 (100%)	619 (95%)	34 (5%)	29	40
1	B	653/653 (100%)	622 (95%)	31 (5%)	32	45
All	All	1306/1306 (100%)	1241 (95%)	65 (5%)	30	43

All (65) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	60	LEU
1	A	73	GLU
1	A	90	LEU
1	A	133	ASP
1	A	142	LEU
1	A	223	LEU
1	A	230	ASP
1	A	236	ILE
1	A	246	LEU
1	A	294	LEU
1	A	300	LEU
1	A	316	LEU
1	A	326	ASP
1	A	343	ARG
1	A	373	LYS
1	A	377	ASN
1	A	385	CYS
1	A	410	LEU
1	A	420	ASN

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Mol	Chain	Res	Type
1	A	431	LEU
1	A	463	LYS
1	A	479	LEU
1	A	482	LEU
1	A	500	LEU
1	A	514	LEU
1	A	543	LEU
1	A	544	LEU
1	A	594	ILE
1	A	660	GLU
1	A	679	ASN
1	A	696	LYS
1	A	715	GLN
1	A	726	VAL
1	A	736	THR
1	B	41	LYS
1	B	49	LEU
1	B	51	ASN
1	B	60	LEU
1	B	66	HIS
1	B	90	LEU
1	B	96	ASP
1	B	129	THR
1	B	140	ARG
1	B	214	LEU
1	B	223	LEU
1	B	230	ASP
1	B	236	ILE
1	B	246	LEU
1	B	358	ARG
1	B	373	LYS
1	B	377	ASN
1	B	385	CYS
1	B	420	ASN
1	B	479	LEU
1	B	507	VAL
1	B	514	LEU
1	B	536	LYS
1	B	543	LEU
1	B	558	VAL
1	B	562	ASN
1	B	566	TYR

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Mol	Chain	Res	Type
1	B	594	ILE
1	B	679	ASN
1	B	684	ARG
1	B	715	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	123	GLN
1	A	169	ASN
1	A	247	GLN
1	A	263	ASN
1	A	298	HIS
1	A	377	ASN
1	A	420	ASN
1	A	483	HIS
1	A	506	ASN
1	A	508	GLN
1	A	533	HIS
1	A	586	GLN
1	A	592	HIS
1	A	679	ASN
1	A	697	GLN
1	A	715	GLN
1	A	750	HIS
1	B	51	ASN
1	B	66	HIS
1	B	75	ASN
1	B	141	GLN
1	B	169	ASN
1	B	263	ASN
1	B	298	HIS
1	B	377	ASN
1	B	383	HIS
1	B	420	ASN
1	B	435	GLN
1	B	483	HIS
1	B	533	HIS
1	B	562	ASN
1	B	612	GLN
1	B	679	ASN
1	B	715	GLN

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Mol	Chain	Res	Type
1	B	750	HIS

### 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](#)

2 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	1WH	A	801	-	26,27,27	1.90	6 (23%)	28,39,39	3.38	13 (46%)
2	1WH	B	801	-	26,27,27	1.71	9 (34%)	28,39,39	2.32	7 (25%)

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	1WH	A	801	-	-	0/9/22/22	0/3/3/3
2	1WH	B	801	-	-	0/9/22/22	0/3/3/3

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	801	1WH	C17-CL1	-4.46	1.64	1.74
2	A	801	1WH	C15-CL	-4.18	1.63	1.73
2	B	801	1WH	C15-CL	-2.28	1.68	1.73
2	B	801	1WH	C17-CL1	-2.24	1.69	1.74
2	B	801	1WH	C18-C19	2.05	1.42	1.38
2	A	801	1WH	C14-C15	2.07	1.44	1.40
2	B	801	1WH	C5-N1	2.11	1.37	1.34
2	B	801	1WH	C14-C15	2.37	1.44	1.40
2	B	801	1WH	C16-C15	2.48	1.42	1.38
2	B	801	1WH	C16-C17	2.51	1.42	1.38
2	A	801	1WH	C18-C19	2.87	1.43	1.38
2	A	801	1WH	C3-C5	2.87	1.42	1.38
2	B	801	1WH	C3-C5	3.25	1.43	1.38
2	A	801	1WH	C18-C17	3.49	1.44	1.38
2	B	801	1WH	C18-C17	3.92	1.45	1.38

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	801	1WH	C16-C17-CL1	-7.55	109.77	119.14
2	A	801	1WH	C16-C15-CL	-7.22	107.37	118.50
2	A	801	1WH	C15-C16-C17	-5.47	112.61	118.69
2	B	801	1WH	C15-C16-C17	-5.25	112.86	118.69
2	A	801	1WH	C8-C7-N2	-4.93	101.90	113.34
2	B	801	1WH	C8-C7-N2	-4.33	103.28	113.34
2	B	801	1WH	C16-C17-CL1	-4.10	114.05	119.14
2	A	801	1WH	C4-C5-C3	-3.14	116.52	122.41
2	A	801	1WH	C1-C3-C5	-3.12	115.88	119.70
2	B	801	1WH	C16-C15-CL	-2.90	114.02	118.50
2	B	801	1WH	C4-C5-C3	-2.37	117.95	122.41
2	A	801	1WH	O2-C-N2	-2.18	119.08	125.13
2	A	801	1WH	O2-C-C7A	2.06	131.87	128.96
2	B	801	1WH	C18-C17-CL1	2.09	122.78	119.35
2	A	801	1WH	C7A-C-N2	2.86	109.05	106.36
2	A	801	1WH	C14-C15-CL	2.91	125.14	120.67
2	A	801	1WH	C2-C7A-C	3.43	133.56	129.69
2	A	801	1WH	C18-C17-CL1	4.16	126.17	119.35
2	B	801	1WH	C16-C15-C14	6.02	126.16	121.76
2	A	801	1WH	C16-C15-C14	7.84	127.48	121.76

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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	728/728 (100%)	0.08	19 (2%) 59 59	34, 47, 69, 84	0
1	B	728/728 (100%)	0.20	26 (3%) 46 45	33, 54, 75, 84	0
All	All	1456/1456 (100%)	0.14	45 (3%) 52 51	33, 50, 73, 84	0

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	39	SER	11.6
1	A	766	PRO	11.3
1	B	279	VAL	5.1
1	B	333	SER	5.0
1	A	765	LEU	4.8
1	B	39	SER	4.6
1	A	342	ALA	4.2
1	B	332	GLU	4.1
1	B	271	VAL	4.1
1	B	766	PRO	3.8
1	B	97	GLU	3.8
1	A	521	GLU	3.7
1	A	142	LEU	3.7
1	B	116	LEU	3.5
1	A	91	GLU	3.2
1	B	140	ARG	3.2
1	B	280	THR	3.1
1	A	98	PHE	3.0
1	A	114	ILE	3.0
1	A	145	GLU	3.0
1	A	90	LEU	2.9
1	A	677	GLU	2.9
1	A	95	PHE	2.9
1	A	279	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	91	GLU	2.7
1	B	273	THR	2.7
1	B	145	GLU	2.7
1	B	521	GLU	2.7
1	B	144	THR	2.6
1	A	393	ASP	2.6
1	A	105	TYR	2.5
1	B	137	LEU	2.4
1	B	765	LEU	2.4
1	B	389	ILE	2.4
1	B	63	ILE	2.4
1	B	330	TYR	2.3
1	B	536	LYS	2.2
1	B	73	GLU	2.1
1	B	114	ILE	2.1
1	A	97	GLU	2.1
1	B	141	GLN	2.1
1	A	89	PHE	2.1
1	A	519	LEU	2.1
1	B	72	GLN	2.0
1	B	615	LYS	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 ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

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
2	1WH	B	801	25/25	0.90	0.26	2.73	55,58,67,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	1WH	A	801	25/25	0.91	0.24	1.53	52,56,63,68	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.