



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:18 AM GMT

PDB ID : 3ABU  
Title : Crystal Structure of LSD1 in complex with a 2-PCPA derivative, S1201  
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Deposited on : 2009-12-21  
Resolution : 3.10 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

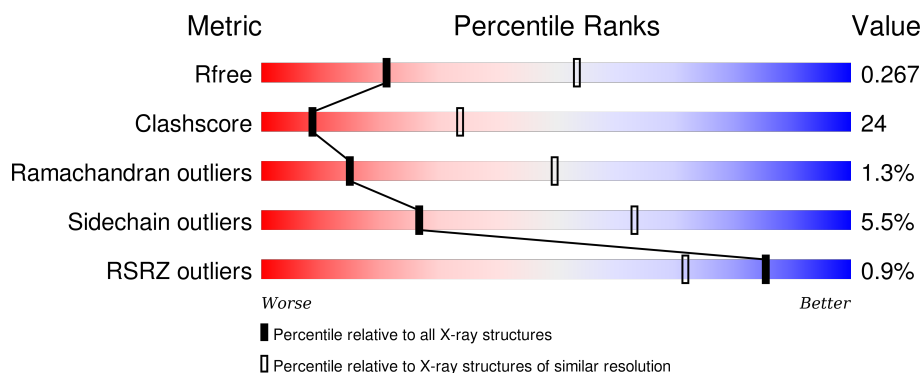
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.10 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	1114 (3.14-3.06)
Clashscore	102246	1222 (3.14-3.06)
Ramachandran outliers	100387	1174 (3.14-3.06)
Sidechain outliers	100360	1174 (3.14-3.06)
RSRZ outliers	91569	1119 (3.14-3.06)

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	662	<div> <div></div> <div>58%</div> <div>35%</div> <div>• •</div> </div>

## 2 Entry composition [i](#)

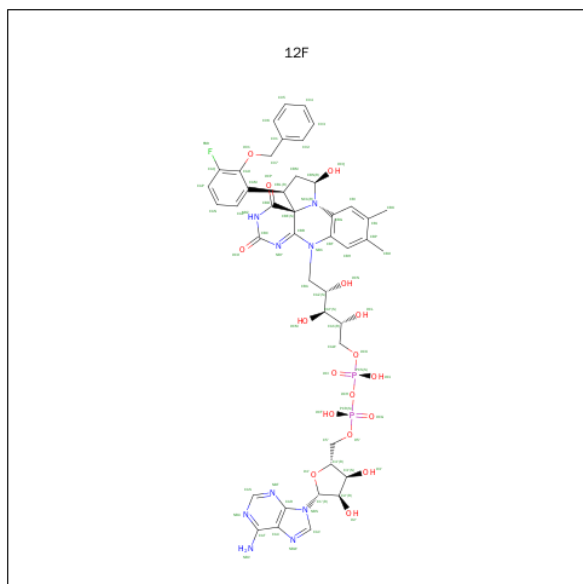
There are 2 unique types of molecules in this entry. The entry contains 5130 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Lysine-specific histone demethylase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	644	5058	3222	879	937	20	0	0	0

- Molecule 2 is [(2R,3S,4R,5R)-5-(6-AMINO-9H-PURIN-9-YL)-3,4-DIHYDROXYTETRAHYDROFURAN-2-YL]METHYL (2R,3S,4S)-5-[(1R,3R,3AS)-3-[2-(BENZYLOXY)-3-FLUOROPHENYL]-1-HYDROXY-10,11-DIMETHYL-4,6-DIOXO-2,3,5,6-TETRAHYDRO-1H-BENZO[G]PYRROLO[2,1-E]PTERIDIN-8(4H)-YL]-2,3,4-TRIHYDROXYPENTYL DIHYDROGEN DIPHOSPHATE (three-letter code: 12F) (formula: C<sub>43</sub>H<sub>48</sub>FN<sub>9</sub>O<sub>17</sub>P<sub>2</sub>).

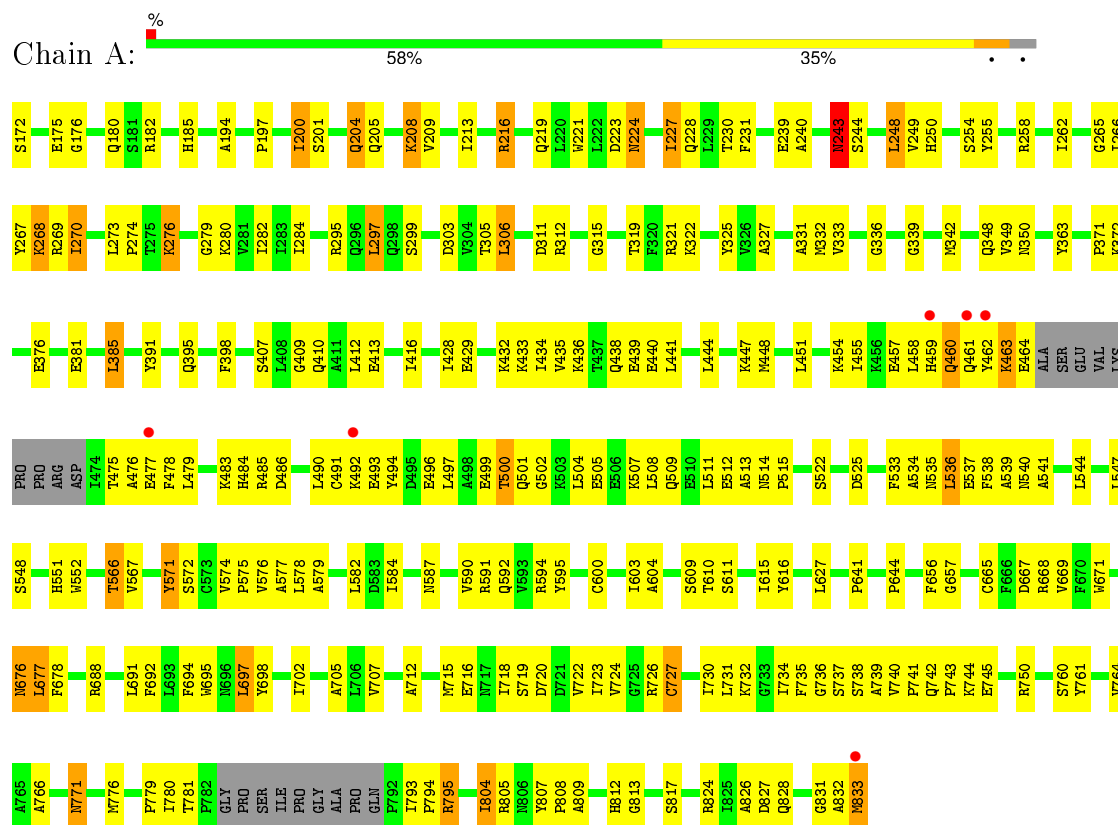


Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	F	N	O	P		
2	A	1	72	43	1	9	17	2	0	0

### 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: Lysine-specific histone demethylase 1



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	183.70Å 183.70Å 109.25Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	47.71 – 3.10 47.71 – 3.10	Depositor EDS
% Data completeness (in resolution range)	100.0 (47.71-3.10) 100.0 (47.71-3.10)	Depositor EDS
$R_{merge}$	0.15	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.67 (at 3.12Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, $R_{free}$	0.242 , 0.295 0.254 , 0.267	Depositor DCC
$R_{free}$ test set	1011 reflections (5.27%)	DCC
Wilson B-factor (Å <sup>2</sup> )	50.5	Xtriage
Anisotropy	0.477	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 38.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.42$ , $\langle L^2 \rangle = 0.25$	Xtriage
Outliers	1 of 364746 reflections (0.000%)	Xtriage
$F_o, F_c$ correlation	0.88	EDS
Total number of atoms	5130	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.52% 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: 12F

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	0.42	0/5163	0.65	0/6994

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5058	0	5091	241	1
2	A	72	0	46	9	0
All	All	5130	0	5137	243	1

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 24.

All (243) 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:537:GLU:HG2	1:A:544:LEU:HD13	1.25	1.09
1:A:276:LYS:HD3	1:A:276:LYS:H	1.14	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:270:ILE:H	1:A:270:ILE:HD13	1.31	0.95
1:A:180:GLN:NE2	1:A:339:GLY:H	1.67	0.91
1:A:391:TYR:CE1	1:A:395:GLN:HG2	2.07	0.90
1:A:172:SER:HB2	1:A:175:GLU:HB3	1.55	0.89
1:A:502:GLY:HA2	1:A:505:GLU:OE2	1.74	0.88
1:A:547:LEU:HD22	1:A:552:TRP:HB2	1.61	0.83
1:A:282:ILE:HD11	1:A:616:TYR:HB3	1.60	0.83
1:A:462:TYR:O	1:A:463:LYS:HB2	1.80	0.81
1:A:781:THR:HG22	1:A:794:PRO:HA	1.66	0.78
1:A:227:ILE:HD11	1:A:270:ILE:CG2	2.14	0.77
1:A:720:ASP:O	1:A:724:VAL:HG23	1.86	0.75
1:A:513:ALA:C	1:A:515:PRO:HD3	2.07	0.74
1:A:460:GLN:O	1:A:461:GLN:HB3	1.88	0.73
1:A:462:TYR:CD2	1:A:483:LYS:HB3	2.22	0.73
1:A:180:GLN:HE22	1:A:339:GLY:H	1.35	0.73
1:A:458:LEU:C	1:A:460:GLN:H	1.93	0.72
1:A:454:LYS:HA	1:A:457:GLU:OE2	1.91	0.70
1:A:269:ARG:HH21	1:A:299:SER:HB2	1.56	0.70
1:A:491:CYS:C	1:A:493:GLU:H	1.95	0.70
1:A:208:LYS:HB2	1:A:208:LYS:NZ	2.08	0.69
1:A:227:ILE:HD11	1:A:270:ILE:HG21	1.74	0.69
1:A:827:ASP:O	1:A:831:GLY:HA2	1.93	0.69
1:A:462:TYR:CZ	1:A:483:LYS:HD2	2.29	0.68
1:A:551:HIS:HB2	1:A:764:VAL:HG11	1.76	0.68
1:A:311:ASP:HB3	1:A:587:ASN:HD21	1.58	0.68
1:A:270:ILE:H	1:A:270:ILE:CD1	2.04	0.67
1:A:276:LYS:N	1:A:276:LYS:HD3	1.99	0.67
1:A:276:LYS:H	1:A:276:LYS:CD	1.93	0.67
1:A:507:LYS:O	1:A:511:LEU:HD13	1.95	0.67
1:A:381:GLU:O	1:A:385:LEU:HD22	1.96	0.66
1:A:804:ILE:O	1:A:804:ILE:HG23	1.96	0.66
1:A:463:LYS:O	1:A:464:GLU:HG3	1.96	0.65
1:A:458:LEU:HD22	1:A:462:TYR:CZ	2.31	0.65
1:A:227:ILE:HD13	1:A:228:GLN:N	2.12	0.64
1:A:205:GLN:O	1:A:209:VAL:HG23	1.97	0.64
1:A:644:PRO:HG2	1:A:780:ILE:HD12	1.78	0.63
1:A:732:LYS:HG2	1:A:737:SER:HA	1.79	0.63
1:A:539:ALA:HA	2:A:1:12F:H03	1.79	0.63
1:A:412:LEU:O	1:A:416:ILE:HG12	1.98	0.63
1:A:274:PRO:HB2	1:A:276:LYS:HE3	1.80	0.63
1:A:282:ILE:CD1	1:A:616:TYR:HB3	2.26	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:719:SER:O	1:A:723:ILE:HG22	1.97	0.63
1:A:270:ILE:HD13	1:A:270:ILE:N	2.08	0.62
1:A:372:LYS:O	1:A:376:GLU:HG3	1.97	0.62
1:A:331:ALA:HA	2:A:1:12F:NCA	2.14	0.62
1:A:227:ILE:HD11	1:A:270:ILE:HG23	1.80	0.62
1:A:311:ASP:CB	1:A:587:ASN:HD21	2.12	0.62
1:A:194:ALA:O	1:A:197:PRO:HD3	2.00	0.62
1:A:266:ILE:HG23	1:A:295:ARG:NH2	2.14	0.62
1:A:544:LEU:HA	1:A:547:LEU:HD12	1.82	0.61
1:A:407:SER:OG	1:A:410:GLN:HB2	2.01	0.61
1:A:455:ILE:HD11	1:A:490:LEU:O	2.00	0.61
1:A:409:GLY:O	1:A:413:GLU:HG2	2.01	0.61
1:A:715:MET:HA	1:A:718:ILE:HD12	1.82	0.61
1:A:332:MET:HG3	1:A:333:VAL:HG23	1.84	0.60
1:A:668:ARG:HH21	1:A:741:PRO:HB3	1.66	0.60
1:A:306:LEU:N	1:A:306:LEU:HD12	2.17	0.60
1:A:230:THR:HG23	1:A:270:ILE:HD11	1.84	0.60
1:A:804:ILE:HD12	1:A:807:TYR:HB2	1.84	0.60
1:A:509:GLN:HA	1:A:512:GLU:OE2	2.02	0.59
1:A:476:ALA:HA	1:A:479:LEU:HB3	1.84	0.59
1:A:499:GLU:C	1:A:501:GLN:H	2.04	0.59
1:A:258:ARG:HD2	1:A:826:ALA:HB3	1.84	0.59
1:A:536:LEU:HD22	1:A:540:ASN:HD22	1.66	0.59
1:A:537:GLU:HG2	1:A:544:LEU:CD1	2.17	0.58
1:A:457:GLU:C	1:A:458:LEU:HD23	2.23	0.58
1:A:541:ALA:HB2	1:A:761:TYR:CZ	2.39	0.58
1:A:268:LYS:HB3	1:A:268:LYS:NZ	2.19	0.57
1:A:508:LEU:O	1:A:512:GLU:HG2	2.05	0.57
1:A:677:LEU:N	1:A:677:LEU:HD23	2.20	0.57
1:A:732:LYS:O	1:A:736:GLY:N	2.35	0.57
1:A:707:VAL:HG12	1:A:712:ALA:HA	1.86	0.57
1:A:665:CYS:HB2	1:A:745:GLU:HB2	1.87	0.57
1:A:566:THR:HG21	1:A:697:LEU:HG	1.87	0.56
1:A:603:ILE:HG13	1:A:615:ILE:HD12	1.86	0.56
1:A:231:PHE:CE1	1:A:250:HIS:HB2	2.41	0.56
1:A:716:GLU:HG2	1:A:750:ARG:HG2	1.86	0.56
1:A:761:TYR:CD2	1:A:809:ALA:HB1	2.40	0.56
1:A:332:MET:CE	1:A:697:LEU:HD21	2.36	0.56
1:A:240:ALA:HA	1:A:243:ASN:ND2	2.21	0.56
1:A:609:SER:O	1:A:611:SER:N	2.39	0.56
1:A:463:LYS:C	1:A:464:GLU:HG3	2.27	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:603:ILE:N	1:A:603:ILE:HD12	2.21	0.55
1:A:208:LYS:HB2	1:A:208:LYS:HZ3	1.69	0.55
1:A:322:LYS:O	1:A:325:TYR:HB2	2.06	0.55
1:A:282:ILE:CD1	1:A:616:TYR:CB	2.85	0.55
1:A:240:ALA:HA	1:A:243:ASN:HD21	1.71	0.55
1:A:274:PRO:CB	1:A:276:LYS:HE3	2.36	0.55
1:A:243:ASN:HD22	1:A:243:ASN:N	2.03	0.55
1:A:567:VAL:HG11	1:A:571:TYR:HA	1.89	0.55
1:A:228:GLN:HB2	1:A:267:TYR:CD2	2.43	0.54
1:A:667:ASP:OD2	1:A:668:ARG:HG3	2.07	0.54
1:A:726:ARG:O	1:A:730:ILE:HG12	2.07	0.54
1:A:221:TRP:CG	1:A:262:ILE:HG22	2.43	0.54
1:A:513:ALA:O	1:A:515:PRO:HD3	2.08	0.53
1:A:536:LEU:HD22	1:A:540:ASN:ND2	2.23	0.53
1:A:491:CYS:C	1:A:493:GLU:N	2.61	0.53
1:A:412:LEU:HD13	1:A:533:PHE:CE1	2.43	0.53
1:A:265:GLY:HA3	1:A:348:GLN:OE1	2.09	0.53
1:A:832:ALA:O	1:A:833:MET:O	2.25	0.53
1:A:477:GLU:O	1:A:477:GLU:HG2	2.08	0.53
1:A:781:THR:HG22	1:A:794:PRO:CA	2.37	0.53
1:A:458:LEU:C	1:A:460:GLN:N	2.61	0.53
1:A:342:MET:HG2	1:A:812:HIS:HB3	1.89	0.52
1:A:363:TYR:CG	1:A:734:ILE:HD12	2.45	0.52
1:A:319:THR:OG1	1:A:572:SER:HB3	2.08	0.52
1:A:231:PHE:CZ	1:A:250:HIS:HB2	2.45	0.52
1:A:197:PRO:HA	1:A:200:ILE:HG22	1.91	0.52
1:A:761:TYR:CZ	2:A:1:12F:HAL	2.44	0.52
1:A:609:SER:C	1:A:611:SER:H	2.13	0.52
1:A:457:GLU:O	1:A:458:LEU:HD23	2.10	0.52
1:A:458:LEU:HD22	1:A:462:TYR:CE1	2.45	0.51
1:A:750:ARG:HG3	1:A:750:ARG:HH11	1.73	0.51
1:A:779:PRO:HG2	1:A:824:ARG:HD3	1.91	0.51
1:A:496:GLU:OE2	1:A:496:GLU:HA	2.11	0.51
1:A:493:GLU:O	1:A:497:LEU:HD13	2.10	0.51
1:A:595:TYR:CZ	1:A:641:PRO:HD2	2.46	0.51
1:A:539:ALA:CB	2:A:1:12F:H03	2.40	0.51
1:A:332:MET:HE2	1:A:697:LEU:HD21	1.92	0.50
1:A:221:TRP:CB	1:A:262:ILE:HG22	2.41	0.50
1:A:243:ASN:ND2	1:A:243:ASN:N	2.57	0.50
1:A:539:ALA:CA	2:A:1:12F:H03	2.41	0.50
1:A:522:SER:N	1:A:525:ASP:HB2	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:807:TYR:O	1:A:813:GLY:HA3	2.12	0.50
1:A:579:ALA:HB1	1:A:584:ILE:CD1	2.42	0.50
1:A:475:THR:HG22	1:A:475:THR:O	2.12	0.50
1:A:807:TYR:N	1:A:808:PRO:CD	2.76	0.49
1:A:719:SER:OG	1:A:722:VAL:HG23	2.12	0.49
1:A:363:TYR:CB	1:A:734:ILE:HD12	2.42	0.49
1:A:460:GLN:O	1:A:461:GLN:CB	2.60	0.49
1:A:321:ARG:HH11	1:A:321:ARG:HG2	1.78	0.49
1:A:295:ARG:HD2	1:A:578:LEU:O	2.13	0.48
1:A:669:VAL:HG13	1:A:671:TRP:CE2	2.48	0.48
1:A:228:GLN:HB2	1:A:267:TYR:CE2	2.47	0.48
1:A:771:ASN:HA	1:A:805:ARG:NH1	2.29	0.48
1:A:776:MET:HE2	1:A:776:MET:HA	1.95	0.48
1:A:533:PHE:O	1:A:537:GLU:HG3	2.14	0.48
1:A:804:ILE:HB	1:A:817:SER:HB3	1.96	0.48
1:A:248:LEU:O	1:A:249:VAL:C	2.52	0.48
1:A:434:ILE:O	1:A:438:GLN:HG3	2.13	0.48
1:A:266:ILE:HD12	1:A:349:VAL:HG12	1.96	0.48
1:A:436:LYS:O	1:A:440:GLU:HG3	2.14	0.48
1:A:760:SER:HA	2:A:1:12F:HBOA	1.95	0.48
1:A:600:CYS:SG	1:A:795:ARG:HG2	2.53	0.47
1:A:325:TYR:HD1	1:A:702:ILE:HD11	1.79	0.47
1:A:175:GLU:HG3	1:A:185:HIS:CD2	2.49	0.47
1:A:734:ILE:HB	1:A:735:PHE:CD2	2.49	0.47
1:A:434:ILE:HD11	1:A:511:LEU:HB3	1.97	0.47
1:A:695:TRP:HB3	1:A:697:LEU:HD13	1.96	0.47
1:A:243:ASN:HD22	1:A:244:SER:N	2.11	0.47
1:A:311:ASP:CA	1:A:587:ASN:HD21	2.28	0.46
1:A:258:ARG:NH1	1:A:827:ASP:OD1	2.48	0.46
1:A:833:MET:N	1:A:833:MET:SD	2.88	0.46
1:A:216:ARG:HA	1:A:216:ARG:HD2	1.71	0.46
1:A:574:VAL:HG12	1:A:575:PRO:N	2.30	0.46
1:A:216:ARG:HE	1:A:219:GLN:NE2	2.14	0.46
1:A:175:GLU:HG3	1:A:185:HIS:CG	2.51	0.46
1:A:512:GLU:H	1:A:512:GLU:HG2	1.48	0.45
1:A:720:ASP:HA	1:A:723:ILE:CG2	2.46	0.45
1:A:514:ASN:N	1:A:515:PRO:HD3	2.32	0.45
1:A:182:ARG:HD2	1:A:807:TYR:OH	2.16	0.45
1:A:441:LEU:HD21	1:A:504:LEU:HB3	1.98	0.45
1:A:312:ARG:HH12	1:A:315:GLY:N	2.14	0.45
1:A:579:ALA:HB1	1:A:584:ILE:HD11	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:223:ASP:O	1:A:224:ASN:HB2	2.17	0.45
1:A:676:ASN:HA	1:A:676:ASN:HD22	1.52	0.45
1:A:603:ILE:HG13	1:A:615:ILE:CD1	2.47	0.45
1:A:761:TYR:CE2	2:A:1:12F:HAL	2.52	0.44
1:A:541:ALA:O	1:A:657:GLY:HA3	2.18	0.44
1:A:579:ALA:HA	1:A:582:LEU:HD12	1.99	0.44
1:A:691:LEU:HD22	1:A:705:ALA:HB1	1.99	0.44
1:A:695:TRP:HB3	1:A:697:LEU:CD1	2.47	0.44
1:A:695:TRP:HE3	1:A:697:LEU:HD11	1.83	0.44
1:A:736:GLY:O	1:A:739:ALA:HB3	2.17	0.44
1:A:429:GLU:O	1:A:433:LYS:HG3	2.17	0.44
1:A:398:PHE:O	1:A:398:PHE:CG	2.71	0.44
2:A:1:12F:HBK	2:A:1:12F:HBO	1.72	0.44
2:A:1:12F:HBM	2:A:1:12F:OCP	2.18	0.44
1:A:435:VAL:O	1:A:439:GLU:HG3	2.18	0.44
1:A:227:ILE:HD13	1:A:227:ILE:C	2.38	0.43
1:A:793:ILE:HD12	1:A:794:PRO:HD2	2.00	0.43
1:A:794:PRO:HD2	1:A:828:GLN:OE1	2.18	0.43
1:A:280:LYS:HD2	1:A:303:ASP:O	2.18	0.43
1:A:548:SER:HA	1:A:766:ALA:HA	1.99	0.43
1:A:476:ALA:C	1:A:478:PHE:H	2.21	0.43
1:A:750:ARG:NH1	1:A:750:ARG:HG3	2.33	0.43
1:A:447:LYS:HD2	1:A:497:LEU:HD21	2.00	0.43
1:A:499:GLU:C	1:A:501:GLN:N	2.71	0.43
1:A:455:ILE:HD11	1:A:490:LEU:HB3	1.99	0.43
1:A:500:THR:O	1:A:504:LEU:HD13	2.18	0.43
1:A:239:GLU:CD	1:A:239:GLU:H	2.22	0.43
1:A:496:GLU:O	1:A:499:GLU:HB3	2.18	0.43
1:A:484:HIS:O	1:A:486:ASP:N	2.52	0.43
1:A:572:SER:O	1:A:576:VAL:HG23	2.19	0.43
1:A:804:ILE:CG2	1:A:804:ILE:O	2.66	0.42
1:A:349:VAL:O	1:A:350:ASN:HB2	2.19	0.42
1:A:243:ASN:HD22	1:A:244:SER:H	1.67	0.42
1:A:737:SER:O	1:A:738:SER:CB	2.67	0.42
1:A:172:SER:O	1:A:176:GLY:N	2.45	0.42
1:A:200:ILE:HG23	1:A:201:SER:N	2.33	0.42
1:A:451:LEU:O	1:A:455:ILE:HD13	2.19	0.42
1:A:462:TYR:CE2	1:A:483:LYS:HD2	2.55	0.42
1:A:567:VAL:HG21	1:A:571:TYR:CG	2.54	0.42
1:A:209:VAL:O	1:A:213:ILE:HG12	2.20	0.42
1:A:200:ILE:O	1:A:200:ILE:HD13	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:428:ILE:CG2	1:A:432:LYS:HE3	2.50	0.42
1:A:727:CYS:O	1:A:731:LEU:HD22	2.20	0.42
1:A:204:GLN:HE21	1:A:204:GLN:HB2	1.63	0.42
1:A:363:TYR:CD2	1:A:734:ILE:HG23	2.53	0.42
1:A:444:LEU:O	1:A:448:MET:HG3	2.20	0.41
1:A:742:GLN:HA	1:A:743:PRO:HD3	1.78	0.41
1:A:732:LYS:HG3	1:A:740:VAL:HB	2.01	0.41
1:A:534:ALA:HB2	1:A:688:ARG:HG3	2.03	0.41
1:A:327:ALA:HA	1:A:698:TYR:CZ	2.55	0.41
1:A:493:GLU:O	1:A:496:GLU:HB3	2.20	0.41
1:A:590:VAL:HA	1:A:604:ALA:HA	2.01	0.41
1:A:248:LEU:HD23	1:A:248:LEU:HA	1.92	0.41
1:A:678:PHE:CE1	1:A:694:PHE:HB2	2.56	0.41
1:A:535:ASN:HA	1:A:692:PHE:CE2	2.56	0.41
1:A:805:ARG:O	1:A:808:PRO:HD3	2.20	0.41
1:A:644:PRO:HG2	1:A:780:ILE:CD1	2.50	0.41
1:A:609:SER:C	1:A:611:SER:N	2.73	0.41
1:A:484:HIS:C	1:A:486:ASP:H	2.24	0.41
1:A:592:GLN:NE2	1:A:594:ARG:HH11	2.19	0.41
1:A:182:ARG:HD2	1:A:807:TYR:CZ	2.56	0.41
1:A:280:LYS:NZ	1:A:305:THR:OG1	2.54	0.41
1:A:227:ILE:HD13	1:A:228:GLN:O	2.21	0.40
1:A:273:LEU:HD21	1:A:299:SER:HA	2.02	0.40
1:A:254:SER:O	1:A:255:TYR:C	2.58	0.40
1:A:494:TYR:C	1:A:496:GLU:N	2.74	0.40
1:A:494:TYR:CD1	1:A:494:TYR:C	2.94	0.40
1:A:484:HIS:C	1:A:486:ASP:N	2.74	0.40
1:A:297:LEU:HD12	1:A:297:LEU:HA	1.87	0.40
1:A:282:ILE:HD13	1:A:616:TYR:HB2	2.03	0.40
1:A:494:TYR:C	1:A:496:GLU:H	2.23	0.40
1:A:371:PRO:O	1:A:372:LYS:C	2.60	0.40
1:A:627:LEU:HD23	1:A:656:PHE:HB2	2.03	0.40
1:A:462:TYR:CD1	1:A:462:TYR:N	2.89	0.40
1:A:266:ILE:CD1	1:A:577:ALA:HB1	2.51	0.40
1:A:492:LYS:O	1:A:492:LYS:HG2	2.20	0.40
1:A:391:TYR:O	1:A:395:GLN:HB3	2.21	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:439:GLU:OE2	1:A:454:LYS:NZ[10_666]	2.13	0.07

## 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	638/662 (96%)	561 (88%)	69 (11%)	8 (1%)	15 50

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	463	LYS
1	A	336	GLY
1	A	610	THR
1	A	243	ASN
1	A	500	THR
1	A	485	ARG
1	A	224	ASN
1	A	279	GLY

### 5.3.2 Protein sidechains [i](#)

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	548/562 (98%)	518 (94%)	30 (6%)	27 63

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	200	ILE
1	A	204	GLN
1	A	208	LYS
1	A	216	ARG
1	A	227	ILE
1	A	243	ASN
1	A	248	LEU
1	A	268	LYS
1	A	270	ILE
1	A	276	LYS
1	A	284	ILE
1	A	297	LEU
1	A	306	LEU
1	A	385	LEU
1	A	459	HIS
1	A	460	GLN
1	A	536	LEU
1	A	538	PHE
1	A	566	THR
1	A	571	TYR
1	A	591	ARG
1	A	676	ASN
1	A	677	LEU
1	A	697	LEU
1	A	727	CYS
1	A	744	LYS
1	A	771	ASN
1	A	795	ARG
1	A	804	ILE
1	A	833	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	180	GLN
1	A	204	GLN
1	A	219	GLN
1	A	237	GLN
1	A	243	ASN
1	A	250	HIS
1	A	259	HIS
1	A	296	GLN
1	A	350	ASN

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Mol	Chain	Res	Type
1	A	368	GLN
1	A	395	GLN
1	A	419	GLN
1	A	430	HIS
1	A	450	ASN
1	A	459	HIS
1	A	461	GLN
1	A	509	GLN
1	A	532	HIS
1	A	540	ASN
1	A	587	ASN
1	A	592	GLN
1	A	638	GLN
1	A	658	ASN
1	A	696	ASN
1	A	742	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](#)

1 ligand is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	12F	A	1	-	72,80,80	1.87	9 (12%)	79,123,123	2.82	13 (16%)

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	12F	A	1	-	-	0/39/111/111	0/8/9/9

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1	12F	CBO-CBP	-5.63	1.39	1.51
2	A	1	12F	CBE-CBL	-2.56	1.53	1.57
2	A	1	12F	CBG-NCA	-2.20	1.33	1.40
2	A	1	12F	O01-C07	-2.11	1.36	1.43
2	A	1	12F	O4'-C1'	2.13	1.43	1.41
2	A	1	12F	CBB-NBY	2.87	1.40	1.31
2	A	1	12F	CAR-NBT	3.26	1.40	1.35
2	A	1	12F	CAS-NBU	7.66	1.48	1.33
2	A	1	12F	CAS-NBT	9.22	1.48	1.32

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1	12F	NBT-CAS-NBU	-21.39	112.52	128.89
2	A	1	12F	C4'-O4'-C1'	-4.63	104.64	109.72
2	A	1	12F	PCS-OCH-PCR	-4.19	120.96	132.73
2	A	1	12F	CAL-CAM-CBL	-3.09	116.39	121.72
2	A	1	12F	CBL-CBM-CBN	-3.04	97.50	104.68
2	A	1	12F	OCP-CBD-CBE	-2.24	119.61	123.76
2	A	1	12F	CAR-CAU-NBW	-2.15	107.50	109.48
2	A	1	12F	CBG-CBF-NBX	2.09	120.89	118.69
2	A	1	12F	FBR-CAQ-CAO	2.13	121.20	117.80
2	A	1	12F	CAS-NBU-CAT	2.22	122.74	118.77
2	A	1	12F	CAO-CAM-CBL	2.80	124.51	120.22
2	A	1	12F	CBE-CBD-NBZ	3.50	121.05	111.03
2	A	1	12F	O01-C07-C01	5.39	125.41	109.21

There are no chirality outliers.

There are no torsion outliers.



There are no ring outliers.

1 monomer is involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1	12F	9	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	644/662 (97%)	-0.19	6 (0%)	85 72	24, 45, 88, 145	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	462	TYR	5.9
1	A	459	HIS	3.9
1	A	833	MET	3.3
1	A	477	GLU	2.5
1	A	492	LYS	2.2
1	A	461	GLN	2.1

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

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

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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( $\text{\AA}^2$ )	Q<0.9
2	12F	A	1	72/72	0.95	0.21	0.22	24,31,35,37	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.