



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 11:58 AM GMT

PDB ID : 3QK5  
Title : Crystal structure of fatty acid amide hydrolase with small molecule inhibitor  
Authors : Min, X.; Walker, N.P.C.; Wang, Z.  
Deposited on : 2011-01-31  
Resolution : 2.20 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.

---

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

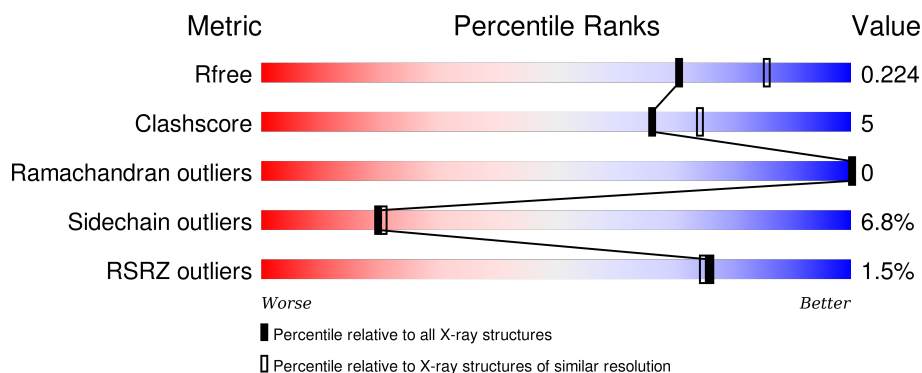
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 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	3774 (2.20-2.20)
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (2.20-2.20)

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	587	 83% 9% • 6%
1	B	587	 79% 12% • 7%

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
3	EDO	A	586	-	-	-	X
3	EDO	B	585	-	-	-	X
3	EDO	B	586	-	-	-	X
3	EDO	B	587	-	-	-	X
3	EDO	B	588	-	-	-	X

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 9545 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 Fatty-acid amide hydrolase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	549	Total	C	N	O	S	0	10	0
			4275	2729	726	789	31			
1	B	546	Total	C	N	O	S	0	10	0
			4255	2716	729	780	30			

There are 78 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	MET	-	EXPRESSION TAG	UNP P97612
A	-6	GLY	-	EXPRESSION TAG	UNP P97612
A	-5	GLY	-	EXPRESSION TAG	UNP P97612
A	-4	SER	-	EXPRESSION TAG	UNP P97612
A	-3	HIS	-	EXPRESSION TAG	UNP P97612
A	-2	HIS	-	EXPRESSION TAG	UNP P97612
A	-1	HIS	-	EXPRESSION TAG	UNP P97612
A	0	HIS	-	EXPRESSION TAG	UNP P97612
A	1	HIS	-	EXPRESSION TAG	UNP P97612
A	2	HIS	-	EXPRESSION TAG	UNP P97612
A	3	GLY	-	EXPRESSION TAG	UNP P97612
A	4	MET	-	EXPRESSION TAG	UNP P97612
A	5	ALA	-	EXPRESSION TAG	UNP P97612
A	6	SER	-	EXPRESSION TAG	UNP P97612
A	7	MET	-	EXPRESSION TAG	UNP P97612
A	8	THR	-	EXPRESSION TAG	UNP P97612
A	9	GLY	-	EXPRESSION TAG	UNP P97612
A	10	GLY	-	EXPRESSION TAG	UNP P97612
A	11	GLN	-	EXPRESSION TAG	UNP P97612
A	12	GLN	-	EXPRESSION TAG	UNP P97612
A	13	MET	-	EXPRESSION TAG	UNP P97612
A	14	GLY	-	EXPRESSION TAG	UNP P97612
A	15	ARG	-	EXPRESSION TAG	UNP P97612
A	16	ASP	-	EXPRESSION TAG	UNP P97612
A	17	LEU	-	EXPRESSION TAG	UNP P97612

*Continued on next page...*

*Continued from previous page...*

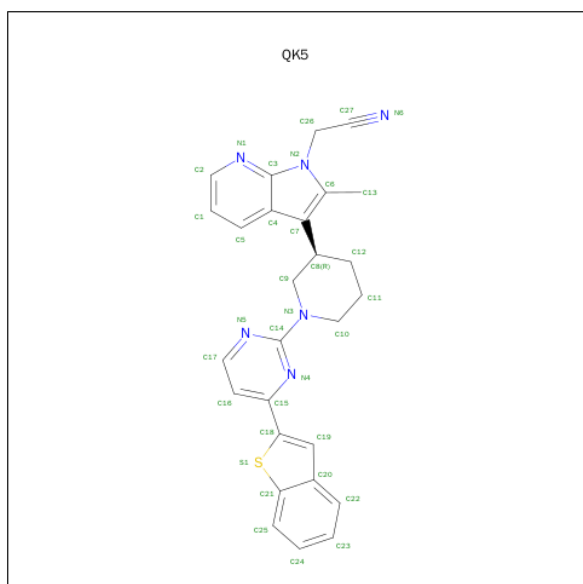
Chain	Residue	Modelled	Actual	Comment	Reference
A	18	TYR	-	EXPRESSION TAG	UNP P97612
A	19	ASP	-	EXPRESSION TAG	UNP P97612
A	20	ASP	-	EXPRESSION TAG	UNP P97612
A	21	ASP	-	EXPRESSION TAG	UNP P97612
A	22	ASP	-	EXPRESSION TAG	UNP P97612
A	23	LYS	-	EXPRESSION TAG	UNP P97612
A	24	ASP	-	EXPRESSION TAG	UNP P97612
A	25	ARG	-	EXPRESSION TAG	UNP P97612
A	26	TRP	-	EXPRESSION TAG	UNP P97612
A	27	GLY	-	EXPRESSION TAG	UNP P97612
A	28	SER	-	EXPRESSION TAG	UNP P97612
A	29	GLU	-	EXPRESSION TAG	UNP P97612
A	30	LEU	-	EXPRESSION TAG	UNP P97612
A	31	GLU	-	EXPRESSION TAG	UNP P97612
B	-7	MET	-	EXPRESSION TAG	UNP P97612
B	-6	GLY	-	EXPRESSION TAG	UNP P97612
B	-5	GLY	-	EXPRESSION TAG	UNP P97612
B	-4	SER	-	EXPRESSION TAG	UNP P97612
B	-3	HIS	-	EXPRESSION TAG	UNP P97612
B	-2	HIS	-	EXPRESSION TAG	UNP P97612
B	-1	HIS	-	EXPRESSION TAG	UNP P97612
B	0	HIS	-	EXPRESSION TAG	UNP P97612
B	1	HIS	-	EXPRESSION TAG	UNP P97612
B	2	HIS	-	EXPRESSION TAG	UNP P97612
B	3	GLY	-	EXPRESSION TAG	UNP P97612
B	4	MET	-	EXPRESSION TAG	UNP P97612
B	5	ALA	-	EXPRESSION TAG	UNP P97612
B	6	SER	-	EXPRESSION TAG	UNP P97612
B	7	MET	-	EXPRESSION TAG	UNP P97612
B	8	THR	-	EXPRESSION TAG	UNP P97612
B	9	GLY	-	EXPRESSION TAG	UNP P97612
B	10	GLY	-	EXPRESSION TAG	UNP P97612
B	11	GLN	-	EXPRESSION TAG	UNP P97612
B	12	GLN	-	EXPRESSION TAG	UNP P97612
B	13	MET	-	EXPRESSION TAG	UNP P97612
B	14	GLY	-	EXPRESSION TAG	UNP P97612
B	15	ARG	-	EXPRESSION TAG	UNP P97612
B	16	ASP	-	EXPRESSION TAG	UNP P97612
B	17	LEU	-	EXPRESSION TAG	UNP P97612
B	18	TYR	-	EXPRESSION TAG	UNP P97612
B	19	ASP	-	EXPRESSION TAG	UNP P97612
B	20	ASP	-	EXPRESSION TAG	UNP P97612

*Continued on next page...*

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	21	ASP	-	EXPRESSION TAG	UNP P97612
B	22	ASP	-	EXPRESSION TAG	UNP P97612
B	23	LYS	-	EXPRESSION TAG	UNP P97612
B	24	ASP	-	EXPRESSION TAG	UNP P97612
B	25	ARG	-	EXPRESSION TAG	UNP P97612
B	26	TRP	-	EXPRESSION TAG	UNP P97612
B	27	GLY	-	EXPRESSION TAG	UNP P97612
B	28	SER	-	EXPRESSION TAG	UNP P97612
B	29	GLU	-	EXPRESSION TAG	UNP P97612
B	30	LEU	-	EXPRESSION TAG	UNP P97612
B	31	GLU	-	EXPRESSION TAG	UNP P97612

- Molecule 2 is (3-{(3R)-1-[4-(1-BENZOTHIOPHEN-2-YL)PYRIMIDIN-2-YL]PIPERIDIN-3-YL}-2-METHYL-1H-PYRROLO[2,3-B]PYRIDIN-1-YL)ACETONITRILE (three-letter code: QK5) (formula: C<sub>27</sub>H<sub>24</sub>N<sub>6</sub>S).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	S	0	0
			34	27	6	1		
2	B	1	Total	C	N	S	0	0
			34	27	6	1		

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



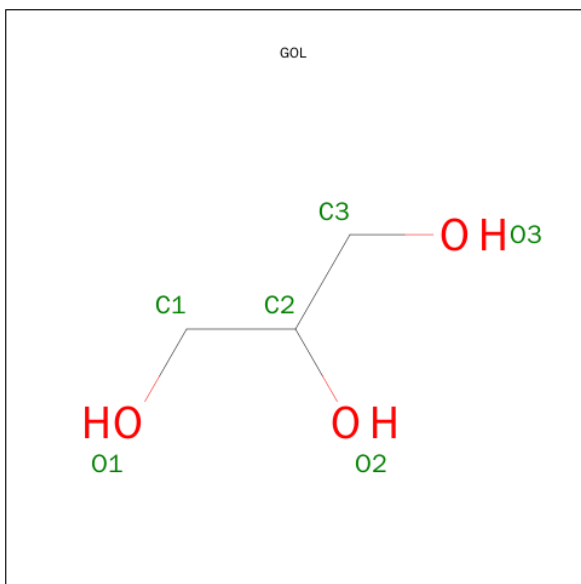
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is water.

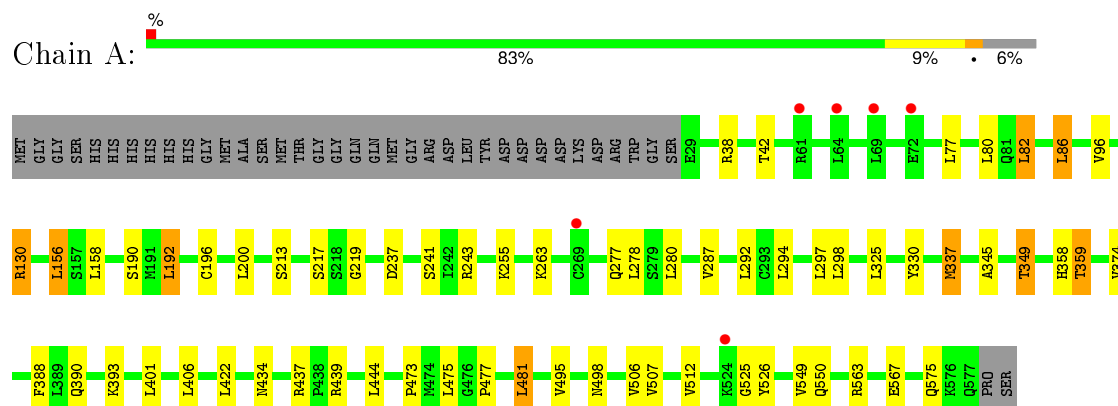
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	410	Total	O	0	0
			410	410		
5	B	471	Total	O	0	0
			471	471		



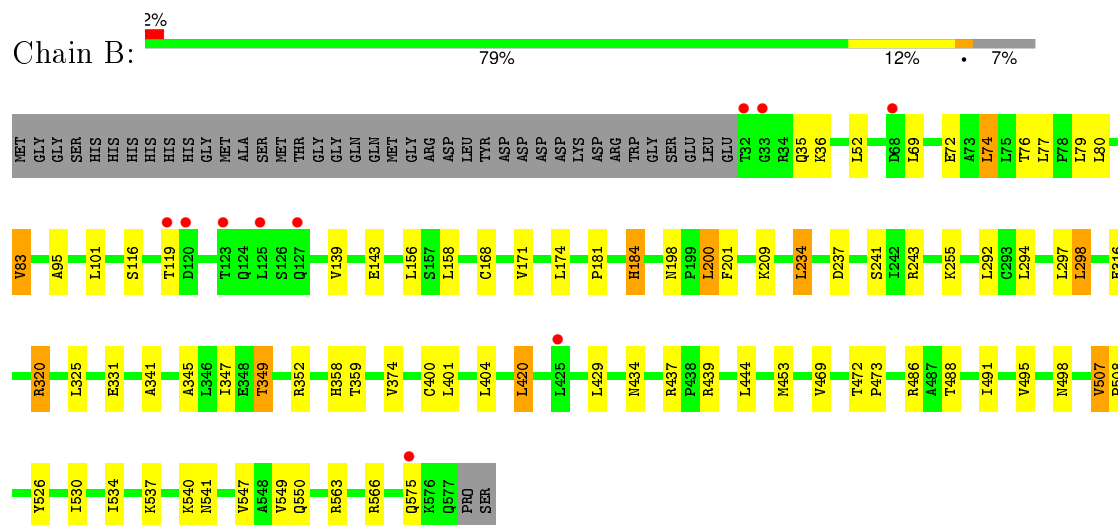
### 3 Residue-property plots [i](#)

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: Fatty-acid amide hydrolase 1



#### • Molecule 1: Fatty-acid amide hydrolase 1



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	91.43Å 104.70Å 148.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.86 – 2.20 29.86 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.2 (29.86-2.20) 99.2 (29.86-2.20)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	0.12	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.59 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.184 , 0.224 0.184 , 0.224	Depositor DCC
$R_{free}$ test set	3648 reflections (5.30%)	DCC
Wilson B-factor (Å <sup>2</sup> )	19.9	Xtriage
Anisotropy	0.123	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 46.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 72433 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	9545	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.50% 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: GOL, EDO, QK5

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	0/4398	0.57	0/5964
1	B	0.39	0/4378	0.58	2/5935 (0.0%)
All	All	0.39	0/8776	0.58	2/11899 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	420	LEU	CA-CB-CG	5.25	127.37	115.30
1	B	74	LEU	CA-CB-CG	5.17	127.18	115.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4275	0	4357	41	0
1	B	4255	0	4349	43	0
2	A	34	0	24	3	0
2	B	34	0	24	1	0
3	A	24	0	36	0	0
3	B	36	0	54	4	0
4	A	6	0	8	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	410	0	0	3	0
5	B	471	0	0	2	0
All	All	9545	0	8852	86	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 5.

All (86) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:352:ARG:HH11	1:B:352:ARG:HG3	1.38	0.89
1:A:325:LEU:H	1:A:358:HIS:HD2	1.17	0.88
1:B:325:LEU:H	1:B:358:HIS:HD2	1.23	0.86
1:B:345:ALA:O	1:B:349:THR:HG23	1.79	0.82
1:A:130:ARG:CG	1:A:130:ARG:HH21	1.95	0.80
1:A:495:VAL:HA	1:A:498:ASN:HD22	1.50	0.77
1:A:263:LYS:HE3	1:A:278:LEU:O	1.89	0.72
1:B:472:THR:HG22	1:B:473:PRO:O	1.89	0.71
1:A:192:LEU:HG	1:A:388:PHE:CE1	2.27	0.70
1:A:130:ARG:HG2	1:A:130:ARG:HH21	1.58	0.68
1:B:198:ASN:HD22	1:B:200:LEU:H	1.40	0.68
1:B:198:ASN:HD21	1:B:201:PHE:H	1.40	0.67
1:B:495:VAL:HA	1:B:498:ASN:HD22	1.61	0.65
1:B:472:THR:HG21	1:B:550:GLN:HE21	1.60	0.64
1:A:325:LEU:H	1:A:358:HIS:CD2	2.09	0.63
1:B:352:ARG:NH1	1:B:352:ARG:HG3	2.11	0.62
1:B:325:LEU:H	1:B:358:HIS:CD2	2.13	0.62
1:A:192:LEU:HD22	2:A:600:QK5:C2	2.30	0.61
1:A:345:ALA:O	1:A:349:THR:HG23	2.00	0.61
1:B:198:ASN:ND2	1:B:201:PHE:H	2.00	0.59
1:B:434:ASN:HD21	1:B:437:ARG:HH11	1.52	0.58
1:A:38:ARG:O	1:A:42:THR:HG23	2.03	0.58
1:A:358:HIS:HE1	1:A:567:GLU:OE1	1.87	0.57
1:A:42:THR:HG21	5:A:978:HOH:O	2.04	0.56
1:A:243:ARG:HH22	1:A:498:ASN:ND2	2.04	0.56
1:B:325:LEU:N	1:B:358:HIS:HD2	2.00	0.56
1:B:434:ASN:ND2	1:B:437:ARG:HH11	2.04	0.55
1:B:79:LEU:O	1:B:83:VAL:HG13	2.07	0.55
1:A:345:ALA:O	1:A:349:THR:CG2	2.55	0.55
1:A:243:ARG:NH2	1:A:498:ASN:HD21	2.06	0.53
2:B:600:QK5:H5	2:B:600:QK5:H12	1.90	0.53

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:168:CYS:SG	1:B:171:VAL:HG23	2.49	0.53
1:B:486:ARG:HB3	1:B:534:ILE:HD13	1.91	0.52
1:B:540:LYS:HD3	3:B:588:EDO:H22	1.91	0.52
1:B:294:LEU:HG	1:B:298:LEU:HD22	1.91	0.51
1:A:243:ARG:HH11	1:A:550:GLN:HE22	1.59	0.51
1:A:243:ARG:HH11	1:A:550:GLN:NE2	2.09	0.51
2:A:600:QK5:H5	2:A:600:QK5:H12	1.93	0.50
1:B:575:GLN:HG2	5:B:880:HOH:O	2.12	0.50
1:A:217:SER:H	1:A:241:SER:CB	2.25	0.49
1:A:390:GLN:HE21	1:A:393:LYS:HE2	1.77	0.49
1:A:477:PRO:HG3	1:A:512:VAL:HG21	1.95	0.49
1:B:341:ALA:HB1	1:B:547:VAL:HG21	1.95	0.49
1:A:359:THR:HG22	5:A:743:HOH:O	2.12	0.48
1:A:337:MET:HG2	1:A:526:TYR:CZ	2.48	0.47
1:A:130:ARG:HH21	1:A:130:ARG:HG3	1.75	0.47
1:B:316:GLU:OE1	1:B:320:ARG:HD2	2.15	0.47
1:A:130:ARG:HD3	1:A:130:ARG:O	2.15	0.47
1:A:434:ASN:HD21	1:A:437:ARG:HH11	1.63	0.47
1:A:190[B]:SER:HG	1:A:388:PHE:HE1	1.62	0.46
1:B:472:THR:CG2	1:B:550:GLN:HE21	2.27	0.45
1:B:453[B]:MET:CE	1:B:453[B]:MET:HA	2.47	0.45
1:A:243:ARG:HD2	1:A:550:GLN:HE21	1.81	0.45
1:A:330:TYR:O	1:A:473:PRO:HD3	2.16	0.45
1:B:69:LEU:HD11	1:B:95:ALA:HB1	1.99	0.44
1:B:243:ARG:NH2	1:B:498:ASN:HD21	2.16	0.44
1:A:390:GLN:HE21	1:A:393:LYS:CE	2.31	0.44
1:A:325:LEU:N	1:A:358:HIS:HD2	1.98	0.44
1:A:196:CYS:SG	1:A:219:GLY:HA3	2.58	0.43
1:B:116:SER:HB3	1:B:184:HIS:HB2	2.00	0.43
1:B:72:GLU:O	1:B:76:THR:HG23	2.19	0.43
1:B:541[B]:ASN:ND2	3:B:588:EDO:H21	2.34	0.42
1:B:139:VAL:O	1:B:181:PRO:HA	2.19	0.42
1:A:213:SER:HA	1:A:481:LEU:HD13	2.02	0.42
1:B:352:ARG:CG	1:B:352:ARG:NH1	2.79	0.42
1:A:434:ASN:ND2	1:A:437:ARG:HH11	2.17	0.42
1:B:36:LYS:HG2	5:B:1020:HOH:O	2.20	0.41
1:B:237:ASP:HB3	1:B:255:LYS:HG3	2.02	0.41
1:A:130:ARG:NH2	1:A:130:ARG:CG	2.65	0.41
1:B:237:ASP:HA	1:B:241:SER:HB2	2.03	0.41
1:A:237:ASP:HB3	1:A:255:LYS:HG3	2.03	0.41
1:B:331:GLU:OE2	1:B:347:ILE:HD11	2.21	0.41

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:429:LEU:HD21	1:B:530:ILE:HG12	2.02	0.41
1:A:337:MET:HB2	1:A:525:GLY:HA2	2.02	0.41
1:A:156:LEU:HB3	1:A:158:LEU:HD23	2.02	0.41
1:B:507:VAL:HA	1:B:508:PRO:HD3	1.96	0.41
1:B:526:TYR:HB3	3:B:583:EDO:H21	2.02	0.41
1:B:488:THR:O	1:B:491:ILE:HG12	2.21	0.41
1:A:82:LEU:HD22	1:A:86:LEU:HD22	2.03	0.41
1:B:174:LEU:HD11	1:B:234:LEU:HD22	2.02	0.41
1:B:566:ARG:HH22	3:B:585:EDO:C2	2.34	0.41
1:A:243:ARG:HD2	1:A:550:GLN:NE2	2.36	0.41
1:A:277:GLN:NE2	5:A:752:HOH:O	2.48	0.41
1:A:192:LEU:HD13	2:A:600:QK5:C1	2.51	0.40
1:B:243:ARG:HH22	1:B:498:ASN:ND2	2.19	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	557/587 (95%)	545 (98%)	12 (2%)	0	100	100
1	B	554/587 (94%)	543 (98%)	11 (2%)	0	100	100
All	All	1111/1174 (95%)	1088 (98%)	23 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 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	476/496 (96%)	445 (94%)	31 (6%)	21	23
1	B	473/496 (95%)	441 (93%)	32 (7%)	20	21
All	All	949/992 (96%)	886 (93%)	63 (7%)	20	22

All (63) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	77	LEU
1	A	80	LEU
1	A	82	LEU
1	A	86	LEU
1	A	96	VAL
1	A	130	ARG
1	A	156	LEU
1	A	192	LEU
1	A	200	LEU
1	A	280	LEU
1	A	287	VAL
1	A	292	LEU
1	A	294	LEU
1	A	297	LEU
1	A	298	LEU
1	A	337	MET
1	A	349	THR
1	A	359	THR
1	A	374	VAL
1	A	401	LEU
1	A	406	LEU
1	A	422	LEU
1	A	439	ARG
1	A	444	LEU
1	A	475	LEU
1	A	481	LEU
1	A	506	VAL
1	A	507	VAL
1	A	549	VAL
1	A	563	ARG
1	A	575	GLN
1	B	35	GLN
1	B	52	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	74	LEU
1	B	77	LEU
1	B	80	LEU
1	B	83	VAL
1	B	101	LEU
1	B	119	THR
1	B	143	GLU
1	B	156	LEU
1	B	158	LEU
1	B	184	HIS
1	B	200	LEU
1	B	234	LEU
1	B	292	LEU
1	B	297	LEU
1	B	298	LEU
1	B	320	ARG
1	B	349	THR
1	B	359	THR
1	B	374	VAL
1	B	400	CYS
1	B	401	LEU
1	B	404	LEU
1	B	420	LEU
1	B	439	ARG
1	B	444	LEU
1	B	469	VAL
1	B	507	VAL
1	B	537	LYS
1	B	549	VAL
1	B	563	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	124	GLN
1	A	127	GLN
1	A	159	ASN
1	A	203	GLN
1	A	259	ASN
1	A	334	ASN
1	A	351	GLN
1	A	358	HIS

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	A	367	ASN
1	A	390	GLN
1	A	434	ASN
1	A	456	GLN
1	A	498	ASN
1	A	550	GLN
1	A	577	GLN
1	B	46	GLN
1	B	124	GLN
1	B	159	ASN
1	B	198	ASN
1	B	259	ASN
1	B	301	HIS
1	B	358	HIS
1	B	391	ASN
1	B	434	ASN
1	B	448	GLN
1	B	498	ASN
1	B	577	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

18 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	$\# Z  > 2$
3	EDO	A	580	-	3,3,3	0.40	0	2,2,2	0.57	0
3	EDO	A	581	-	3,3,3	0.44	0	2,2,2	0.40	0
3	EDO	A	582	-	3,3,3	0.47	0	2,2,2	0.41	0
4	GOL	A	583	-	5,5,5	0.44	0	5,5,5	0.12	0
3	EDO	A	584	-	3,3,3	0.44	0	2,2,2	0.47	0
3	EDO	A	585	-	3,3,3	0.48	0	2,2,2	0.37	0
3	EDO	A	586	-	3,3,3	0.49	0	2,2,2	0.39	0
2	QK5	A	600	-	33,39,39	1.40	5 (15%)	36,56,56	2.18	11 (30%)
3	EDO	B	580	-	3,3,3	0.50	0	2,2,2	0.33	0
3	EDO	B	581	-	3,3,3	0.46	0	2,2,2	0.43	0
3	EDO	B	582	-	3,3,3	0.49	0	2,2,2	0.39	0
3	EDO	B	583	-	3,3,3	0.49	0	2,2,2	0.38	0
3	EDO	B	584	-	3,3,3	0.49	0	2,2,2	0.37	0
3	EDO	B	585	-	3,3,3	0.46	0	2,2,2	0.47	0
3	EDO	B	586	-	3,3,3	0.48	0	2,2,2	0.41	0
3	EDO	B	587	-	3,3,3	0.44	0	2,2,2	0.51	0
3	EDO	B	588	-	3,3,3	0.54	0	2,2,2	0.21	0
2	QK5	B	600	-	33,39,39	1.35	4 (12%)	36,56,56	2.22	11 (30%)

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
3	EDO	A	580	-	-	0/1/1/1	0/0/0/0
3	EDO	A	581	-	-	0/1/1/1	0/0/0/0
3	EDO	A	582	-	-	0/1/1/1	0/0/0/0
4	GOL	A	583	-	-	0/4/4/4	0/0/0/0
3	EDO	A	584	-	-	0/1/1/1	0/0/0/0
3	EDO	A	585	-	-	0/1/1/1	0/0/0/0
3	EDO	A	586	-	-	0/1/1/1	0/0/0/0
2	QK5	A	600	-	-	0/6/25/25	0/6/6/6
3	EDO	B	580	-	-	0/1/1/1	0/0/0/0
3	EDO	B	581	-	-	0/1/1/1	0/0/0/0
3	EDO	B	582	-	-	0/1/1/1	0/0/0/0
3	EDO	B	583	-	-	0/1/1/1	0/0/0/0
3	EDO	B	584	-	-	0/1/1/1	0/0/0/0
3	EDO	B	585	-	-	0/1/1/1	0/0/0/0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	B	586	-	-	0/1/1/1	0/0/0/0
3	EDO	B	587	-	-	0/1/1/1	0/0/0/0
3	EDO	B	588	-	-	0/1/1/1	0/0/0/0
2	QK5	B	600	-	-	0/6/25/25	0/6/6/6

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	600	QK5	C15-C18	-4.25	1.39	1.49
2	B	600	QK5	C15-C18	-4.11	1.39	1.49
2	A	600	QK5	C6-N2	-2.55	1.34	1.39
2	B	600	QK5	C6-N2	-2.50	1.34	1.39
2	A	600	QK5	C18-S1	-2.24	1.69	1.72
2	B	600	QK5	C13-C6	2.07	1.54	1.49
2	A	600	QK5	C10-N3	2.19	1.50	1.46
2	B	600	QK5	C14-N3	2.69	1.40	1.35
2	A	600	QK5	C14-N3	3.00	1.41	1.35

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	600	QK5	N5-C14-N4	-6.13	119.76	126.30
2	B	600	QK5	N5-C14-N4	-5.73	120.19	126.30
2	B	600	QK5	C16-C17-N5	-3.34	120.08	123.90
2	A	600	QK5	C16-C17-N5	-3.05	120.42	123.90
2	B	600	QK5	C19-C18-S1	-2.65	107.91	110.75
2	B	600	QK5	C16-C15-N4	-2.55	118.49	122.01
2	A	600	QK5	C13-C6-C7	-2.42	124.93	128.68
2	B	600	QK5	C13-C6-C7	-2.23	125.22	128.68
2	A	600	QK5	C19-C18-S1	-2.22	108.37	110.75
2	A	600	QK5	C7-C6-N2	2.24	108.21	106.70
2	A	600	QK5	C10-N3-C9	2.82	119.22	113.30
2	B	600	QK5	C13-C6-N2	3.03	126.83	122.82
2	A	600	QK5	C13-C6-N2	3.06	126.86	122.82
2	B	600	QK5	C10-N3-C9	3.15	119.90	113.30
2	A	600	QK5	C19-C20-C21	3.29	113.55	107.04
2	B	600	QK5	C19-C20-C21	3.30	113.57	107.04
2	B	600	QK5	C17-N5-C14	3.83	120.68	115.21
2	A	600	QK5	C2-N1-C3	3.84	121.70	116.93
2	B	600	QK5	C2-N1-C3	3.87	121.73	116.93
2	A	600	QK5	C17-N5-C14	4.02	120.95	115.21
2	A	600	QK5	N5-C14-N3	5.09	121.82	116.89

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	600	QK5	N5-C14-N3	5.29	122.01	116.89

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	600	QK5	3	0
3	B	583	EDO	1	0
3	B	585	EDO	1	0
3	B	588	EDO	2	0
2	B	600	QK5	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

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

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

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	549/587 (93%)	-0.18	6 (1%) 82 82	14, 21, 33, 48	0
1	B	546/587 (93%)	-0.18	10 (1%) 71 70	12, 19, 34, 42	0
All	All	1095/1174 (93%)	-0.18	16 (1%) 76 75	12, 20, 34, 48	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	32	THR	7.0
1	A	72	GLU	4.0
1	B	123	THR	3.6
1	B	33	GLY	3.2
1	B	127	GLN	3.2
1	B	575	GLN	3.1
1	B	425	LEU	2.7
1	B	125	LEU	2.6
1	B	120	ASP	2.5
1	B	119	THR	2.4
1	A	269	CYS	2.4
1	A	61	ARG	2.4
1	A	64	LEU	2.3
1	A	69	LEU	2.2
1	A	524	LYS	2.1
1	B	68	ASP	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 ⓘ

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
3	EDO	B	585	4/4	0.80	0.47	12.78	45,45,45,45	0
3	EDO	B	588	4/4	0.58	0.35	6.89	33,35,35,35	0
3	EDO	A	586	4/4	0.72	0.37	3.71	54,54,54,54	0
3	EDO	B	587	4/4	0.83	0.31	2.86	60,60,60,60	0
3	EDO	B	586	4/4	0.61	0.22	2.09	44,44,44,44	0
4	GOL	A	583	6/6	0.68	0.26	1.99	35,36,38,38	0
3	EDO	B	580	4/4	0.73	0.18	1.99	40,40,40,40	0
2	QK5	A	600	34/34	0.88	0.16	1.73	27,28,31,31	0
2	QK5	B	600	34/34	0.86	0.17	1.52	25,28,31,31	0
3	EDO	A	585	4/4	0.85	0.15	1.12	40,40,40,41	0
3	EDO	B	584	4/4	0.84	0.14	0.96	41,41,42,42	0
3	EDO	A	584	4/4	0.81	0.15	0.50	47,48,48,48	0
3	EDO	A	581	4/4	0.86	0.12	0.21	35,35,35,36	0
3	EDO	B	583	4/4	0.71	0.17	-	45,45,45,46	0
3	EDO	A	582	4/4	0.89	0.12	-	43,43,43,43	0
3	EDO	B	581	4/4	0.91	0.14	-	34,34,34,34	0
3	EDO	B	582	4/4	0.50	0.30	-	48,48,49,49	0
3	EDO	A	580	4/4	0.84	0.22	-	42,42,42,42	0

### 6.5 Other polymers ⓘ

There are no such residues in this entry.