



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 09:02 PM GMT

PDB ID : 1N95
Title : Aryl Tetrahydrophyridine Inhibitors of Farnesyltransferase: Glycine, Phenylalanine and Histidine Derivatives
Authors : Gwaltney II, S.L.; O'Conner, S.J.; Nelson, L.T.; Sullivan, G.M.; Imade, H.; Wang, W.; Hasvold, L.; Li, Q.; Cohen, J.; Gu, W.Z.
Deposited on : 2002-11-22
Resolution : 2.30 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
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

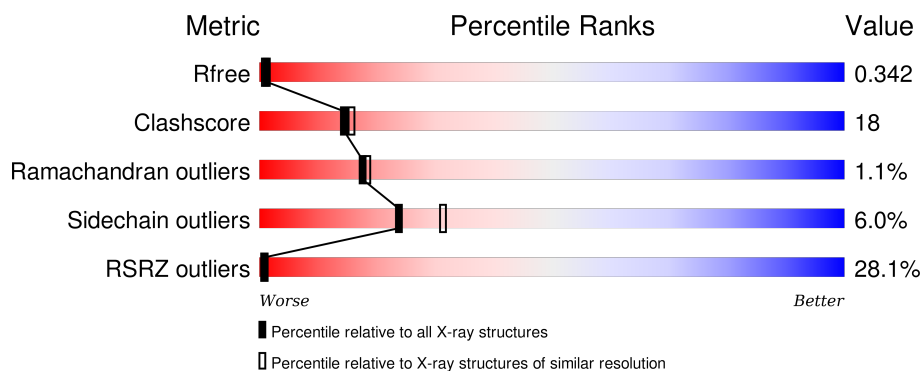
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (2.30-2.30)

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 ≥ 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	315	
2	B	402	

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
4	HFP	B	501	X	-	X	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 5873 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 Protein farnesyltransferase alpha subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	312	Total	C	N	O	S	0	0	0
			2660	1695	465	495	5			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	156	THR	ILE	CONFLICT	UNP Q04631

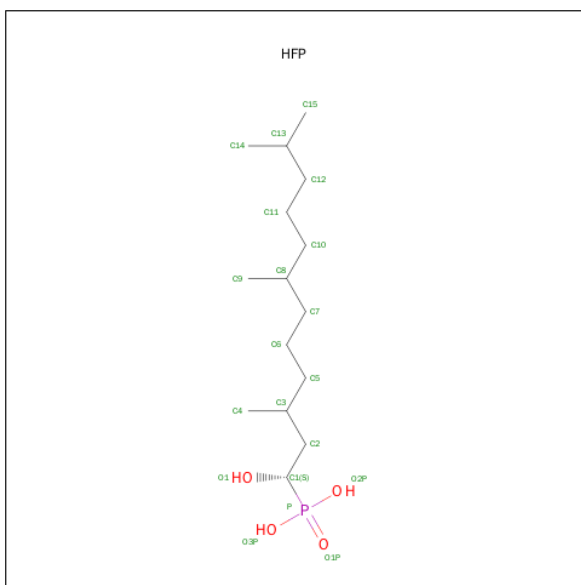
- Molecule 2 is a protein called Protein farnesyltransferase beta subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	401	Total	C	N	O	S	0	0	0
			3154	2016	543	572	23			

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

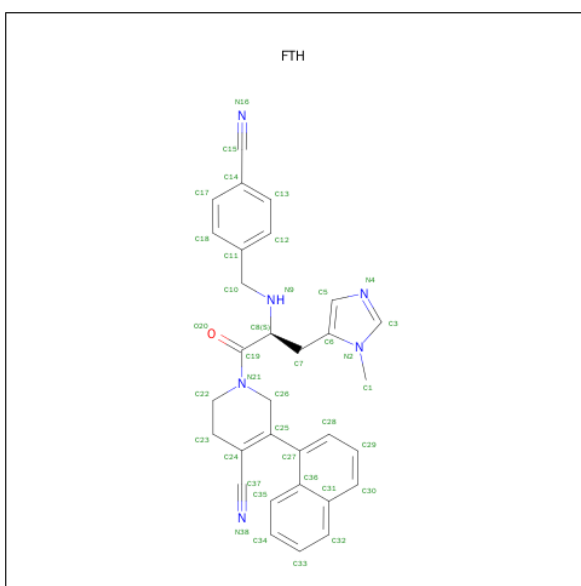
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Zn	0	0
			1	1		

- Molecule 4 is ALPHA-HYDROXYFARNESYLPHOSPHONIC ACID (three-letter code: HFP) (formula: C₁₅H₃₃O₄P).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total	C	O	P	0	0
			20	15	4	1		

- Molecule 5 is 1-[2-(4-CYANO-BENZYLAMINO)-3-(3-METHYL-3H-IMIDAZOL-4-YL)-PROPIONYL]-5-NAPHTHALEN-1-YL-1,2,3,6-TETRAHYDRO-PYRIDINE-4-CARBONITRILE (three-letter code: FTH) (formula: $C_{31}H_{28}N_6O$).

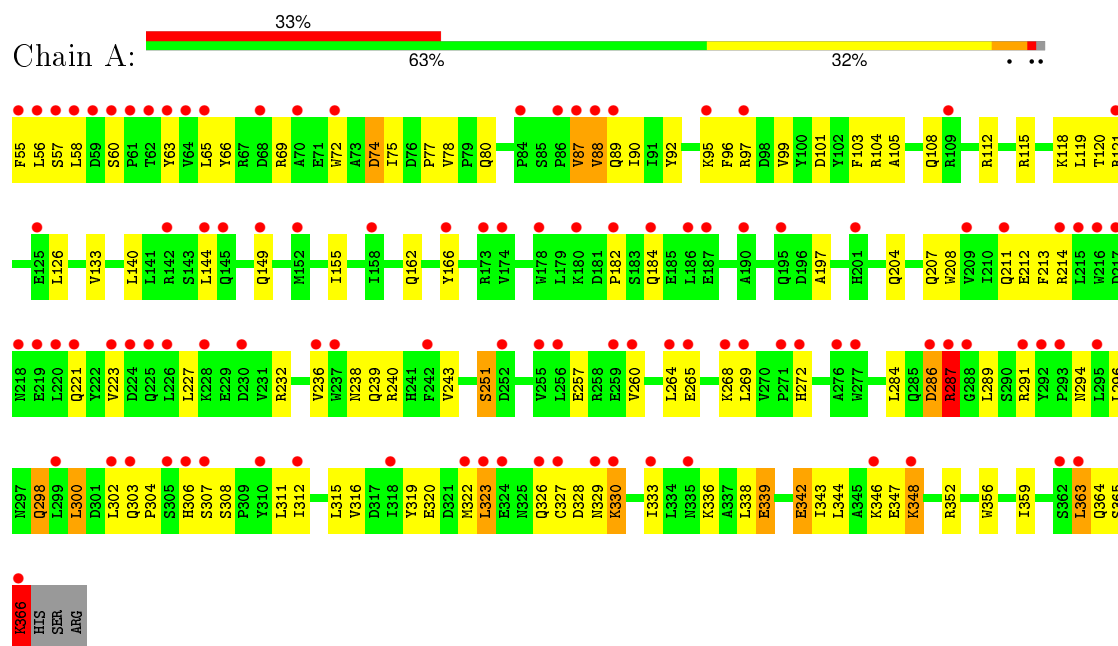


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	1	Total	C	N	O	0	0
			38	31	6	1		

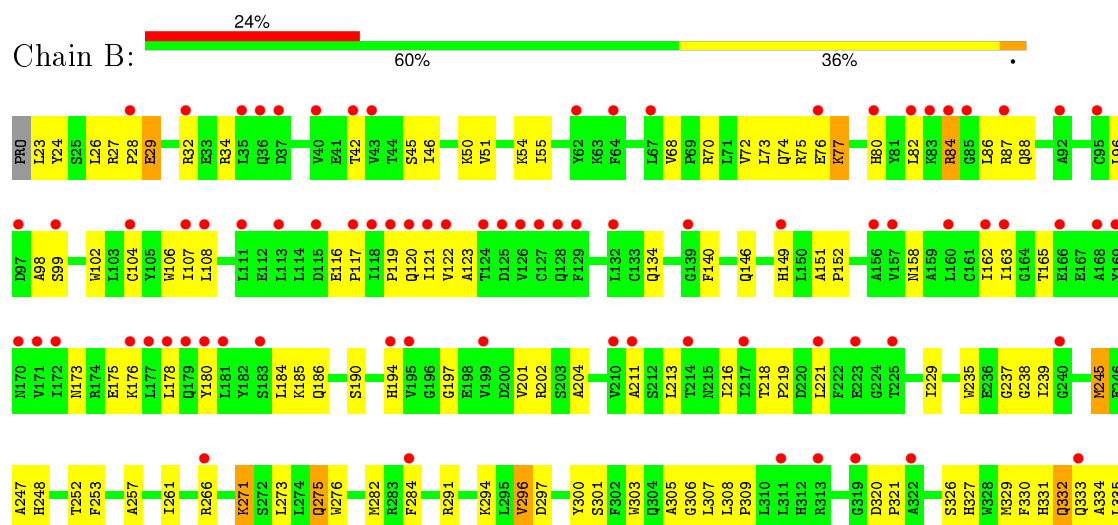
3 Residue-property plots

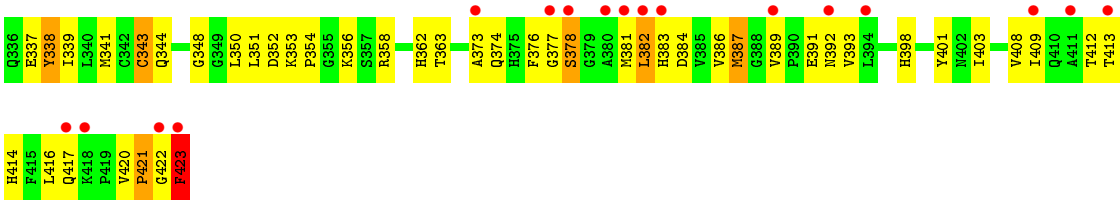
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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: Protein farnesyltransferase alpha subunit



- Molecule 2: Protein farnesyltransferase beta subunit





4 Data and refinement statistics

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α , β , γ	171.13 Å 171.13 Å 69.40 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	43.59 – 2.30 43.59 – 2.30	Depositor EDS
% Data completeness (in resolution range)	(Not available) (43.59-2.30) 83.5 (43.59-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.33 (at 2.29 Å)	Xtriage
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.337 , 0.358 0.321 , 0.342	Depositor DCC
R_{free} test set	4340 reflections (10.05%)	DCC
Wilson B-factor (Å ²)	29.5	Xtriage
Anisotropy	0.241	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 26.4	EDS
Estimated twinning fraction	0.030 for h,-h-k,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	1 of 49954 reflections (0.002%)	Xtriage
F_o, F_c correlation	0.84	EDS
Total number of atoms	5873	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.12% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: HFP, ZN, FTH

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	0.59	1/2725 (0.0%)	0.83	4/3700 (0.1%)
2	B	0.60	3/3239 (0.1%)	0.83	1/4397 (0.0%)
All	All	0.60	4/5964 (0.1%)	0.83	5/8097 (0.1%)

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
2	B	0	1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	343	CYS	CB-SG	-7.00	1.70	1.82
2	B	423	PHE	C-O	6.61	1.35	1.23
2	B	423	PHE	C-OXT	6.03	1.34	1.23
1	A	366	LYS	CA-CB	6.00	1.67	1.53

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
2	B	423	PHE	CA-C-O	23.35	169.13	120.10
1	A	366	LYS	CA-C-O	15.64	152.94	120.10
1	A	287	ARG	NE-CZ-NH1	-14.37	113.11	120.30
1	A	74	ASP	CB-CG-OD1	-9.70	109.57	118.30
1	A	74	ASP	CB-CG-OD2	5.60	123.34	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	338	TYR	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2660	0	2585	82	3
2	B	3154	0	3085	123	2
3	B	1	0	0	0	0
4	B	20	0	28	10	0
5	B	38	0	28	14	0
All	All	5873	0	5726	209	3

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 18.

All (209) 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:B:245:MET:HE3	2:B:245:MET:HA	1.52	0.91
2:B:77:LYS:HA	2:B:77:LYS:HE3	1.53	0.90
2:B:271:LYS:HE3	2:B:271:LYS:HA	1.54	0.87
2:B:84:ARG:HH22	2:B:88:GLN:HG2	1.40	0.83
2:B:218:THR:HB	2:B:219:PRO:HD2	1.62	0.81
2:B:185:LYS:HE3	2:B:221:LEU:O	1.82	0.79
1:A:322:MET:HE3	1:A:333:ILE:HD13	1.65	0.79
2:B:106:TRP:CH2	5:B:1001:FTH:HC13	2.20	0.76
1:A:312:ILE:O	1:A:316:VAL:HG23	1.86	0.75
2:B:178:LEU:HD12	2:B:421:PRO:HB2	1.68	0.74
2:B:116:GLU:HB3	2:B:117:PRO:HD2	1.70	0.73
1:A:287:ARG:HD3	1:A:291:ARG:HD3	1.71	0.72
2:B:84:ARG:NH2	2:B:88:GLN:HG2	2.05	0.71
2:B:178:LEU:HG	2:B:216:ILE:HB	1.72	0.71
2:B:338:TYR:CE2	2:B:343:CYS:SG	2.86	0.69
2:B:151:ALA:HB3	2:B:152:PRO:HD3	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:327:CYS:O	1:A:330:LYS:HB3	1.93	0.67
2:B:73:LEU:O	2:B:75:ARG:N	2.28	0.66
2:B:253:PHE:HA	2:B:307:LEU:HD21	1.78	0.66
2:B:82:LEU:HD21	2:B:363:THR:HG21	1.78	0.66
1:A:365:SER:HB2	1:A:366:LYS:HD3	1.77	0.66
1:A:344:LEU:HD23	1:A:348:LYS:HB3	1.78	0.65
1:A:268:LYS:HE2	1:A:302:LEU:HD11	1.79	0.65
1:A:343:ILE:HG22	1:A:348:LYS:HB2	1.78	0.64
1:A:312:ILE:HD12	1:A:348:LYS:HG2	1.79	0.63
1:A:303:GLN:O	1:A:307:SER:HB2	1.98	0.63
1:A:302:LEU:HD22	1:A:306:HIS:CD2	2.33	0.63
2:B:72:VAL:HG22	2:B:389:VAL:HG21	1.80	0.63
2:B:335:LEU:O	2:B:339:ILE:HG13	1.99	0.63
2:B:96:LEU:HD11	5:B:1001:FTH:C14	2.29	0.63
2:B:301:SER:O	2:B:305:ALA:HB3	1.98	0.63
1:A:223:VAL:HG11	1:A:240:ARG:HB2	1.81	0.62
2:B:327:HIS:HB3	2:B:332:GLN:HE22	1.64	0.62
2:B:73:LEU:HD12	2:B:344:GLN:OE1	1.99	0.62
2:B:353:LYS:HB2	2:B:354:PRO:HD2	1.81	0.61
1:A:80:GLN:HB2	1:A:104:ARG:CZ	2.31	0.61
2:B:51:VAL:HA	2:B:54:LYS:HE2	1.83	0.59
2:B:308:LEU:HD13	2:B:330:PHE:HB3	1.84	0.59
2:B:239:ILE:HB	2:B:252:THR:HA	1.85	0.59
1:A:359:ILE:O	1:A:363:LEU:HB2	2.02	0.59
2:B:96:LEU:HD11	5:B:1001:FTH:C15	2.32	0.59
2:B:73:LEU:H	2:B:392:ASN:ND2	2.00	0.58
2:B:352:ASP:HB3	2:B:356:LYS:HG3	1.86	0.58
4:B:501:HFP:H52	5:B:1001:FTH:H231	1.85	0.58
1:A:347:GLU:HG2	1:A:348:LYS:HE3	1.85	0.58
2:B:180:TYR:CZ	2:B:184:LEU:HD11	2.38	0.58
1:A:208:TRP:NE1	1:A:212:GLU:HG3	2.20	0.57
2:B:104:CYS:O	2:B:108:LEU:HB2	2.05	0.57
2:B:308:LEU:CD1	2:B:330:PHE:HB3	2.35	0.57
2:B:282:MET:CG	2:B:296:VAL:HG13	2.34	0.57
4:B:501:HFP:C5	5:B:1001:FTH:H231	2.35	0.57
2:B:98:ALA:HA	2:B:146:GLN:HE22	1.69	0.56
1:A:342:GLU:OE1	1:A:346:LYS:HE3	2.06	0.56
1:A:366:LYS:N	1:A:366:LYS:HD3	2.21	0.56
1:A:55:PHE:HB2	1:A:118:LYS:HD3	1.87	0.56
1:A:319:TYR:HD2	1:A:322:MET:HE2	1.71	0.55
1:A:286:ASP:O	1:A:287:ARG:HB2	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:104:ARG:O	1:A:108:GLN:HB2	2.05	0.55
1:A:87:VAL:O	1:A:88:VAL:C	2.43	0.55
1:A:90:ILE:HB	1:A:92:TYR:CE2	2.42	0.55
1:A:149:GLN:HE22	1:A:184:GLN:HE22	1.54	0.55
2:B:282:MET:HG3	2:B:296:VAL:HG13	1.89	0.55
1:A:338:LEU:HD11	1:A:364:GLN:HE22	1.72	0.55
2:B:72:VAL:HG22	2:B:389:VAL:CG2	2.37	0.55
2:B:75:ARG:NH2	2:B:391:GLU:O	2.40	0.54
2:B:257:ALA:O	2:B:261:ILE:HG13	2.07	0.54
2:B:386:VAL:HG21	2:B:393:VAL:HB	1.89	0.54
1:A:294:ASN:O	1:A:298:GLN:HG2	2.06	0.54
2:B:374:GLN:O	2:B:384:ASP:HA	2.08	0.54
2:B:398:HIS:CD2	2:B:408:VAL:HG11	2.42	0.54
2:B:326:SER:O	2:B:383:HIS:HB3	2.08	0.53
2:B:362:HIS:CE1	5:B:1001:FTH:N4	2.77	0.53
1:A:356:TRP:HA	1:A:356:TRP:CE3	2.44	0.53
2:B:202:ARG:HD3	5:B:1001:FTH:N38	2.23	0.53
2:B:84:ARG:HH22	2:B:88:GLN:CG	2.17	0.53
1:A:75:ILE:HD11	1:A:115:ARG:CZ	2.39	0.53
2:B:86:LEU:HB2	2:B:107:ILE:HG21	1.90	0.53
2:B:381:MET:O	2:B:382:LEU:HD22	2.09	0.53
2:B:337:GLU:HB3	2:B:341:MET:HE3	1.91	0.52
4:B:501:HFP:H112	5:B:1001:FTH:C28	2.39	0.52
1:A:287:ARG:HD3	1:A:287:ARG:O	2.09	0.52
2:B:50:LYS:O	2:B:54:LYS:HG3	2.09	0.52
2:B:398:HIS:CD2	2:B:408:VAL:HG21	2.44	0.52
1:A:96:PHE:HA	1:A:126:LEU:HD13	1.93	0.51
2:B:186:GLN:HB2	2:B:190:SER:O	2.10	0.51
1:A:223:VAL:HG13	1:A:236:VAL:HG12	1.93	0.51
2:B:46:ILE:HG22	2:B:50:LYS:HE3	1.93	0.51
1:A:72:TRP:CE3	1:A:75:ILE:HD12	2.45	0.51
2:B:76:GLU:O	2:B:80:HIS:ND1	2.44	0.51
2:B:158:ASN:O	2:B:162:ILE:HG13	2.12	0.50
2:B:414:HIS:O	2:B:417:GLN:HG2	2.11	0.50
2:B:348:GLY:O	2:B:358:ARG:HD2	2.11	0.50
1:A:302:LEU:HD22	1:A:306:HIS:HD2	1.74	0.50
1:A:296:LEU:O	1:A:300:LEU:HB2	2.11	0.50
1:A:103:PHE:CZ	1:A:133:VAL:HG22	2.46	0.50
2:B:275:GLN:HE21	2:B:276:TRP:N	2.10	0.50
1:A:78:VAL:HG23	1:A:105:ALA:HB2	1.94	0.50
2:B:245:MET:CE	2:B:245:MET:HA	2.35	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:328:ASP:O	1:A:329:ASN:HB2	2.12	0.50
2:B:344:GLN:HA	2:B:350:LEU:HD13	1.93	0.50
2:B:297:ASP:HB3	2:B:300:TYR:HD1	1.76	0.49
2:B:412:THR:O	2:B:416:LEU:HB2	2.12	0.49
2:B:23:LEU:O	2:B:27:ARG:HG3	2.12	0.49
2:B:389:VAL:HG12	2:B:391:GLU:HB2	1.94	0.48
2:B:350:LEU:HB2	2:B:363:THR:HA	1.95	0.48
1:A:182:PRO:HG3	1:A:213:PHE:CD2	2.49	0.48
1:A:227:LEU:HG	1:A:236:VAL:CG1	2.44	0.48
2:B:73:LEU:H	2:B:392:ASN:HD21	1.62	0.48
1:A:89:GLN:OE1	2:B:87:ARG:NH2	2.47	0.48
2:B:23:LEU:HD12	2:B:26:LEU:CD1	2.44	0.48
1:A:238:ASN:HA	2:B:235:TRP:CZ2	2.50	0.47
2:B:326:SER:HB2	2:B:383:HIS:CD2	2.49	0.47
2:B:121:ILE:N	2:B:121:ILE:HD12	2.30	0.47
1:A:312:ILE:HG22	1:A:344:LEU:HD11	1.96	0.47
2:B:216:ILE:HG22	2:B:421:PRO:CD	2.44	0.47
1:A:311:LEU:O	1:A:315:LEU:HG	2.14	0.47
2:B:308:LEU:HD22	2:B:329:MET:HB2	1.97	0.47
2:B:51:VAL:O	2:B:55:ILE:HG12	2.15	0.47
2:B:376:PHE:CZ	2:B:378:SER:HB2	2.50	0.46
2:B:119:PRO:O	2:B:122:VAL:HG12	2.15	0.46
2:B:134:GLN:HB2	2:B:140:PHE:CE2	2.51	0.46
2:B:55:ILE:HD13	2:B:354:PRO:HG3	1.98	0.46
1:A:92:TYR:HB2	1:A:97:ARG:HG3	1.98	0.46
1:A:80:GLN:HB2	1:A:104:ARG:NH2	2.31	0.45
2:B:108:LEU:O	2:B:162:ILE:HG21	2.17	0.45
1:A:312:ILE:CD1	1:A:348:LYS:HG2	2.45	0.45
2:B:378:SER:HB3	2:B:381:MET:HG3	1.99	0.45
2:B:423:PHE:CD2	2:B:423:PHE:N	2.84	0.45
1:A:300:LEU:HA	1:A:300:LEU:HD12	1.81	0.45
2:B:306:GLY:O	2:B:309:PRO:HD2	2.17	0.45
1:A:264:LEU:HD23	1:A:264:LEU:HA	1.86	0.45
2:B:218:THR:HB	2:B:219:PRO:CD	2.42	0.44
2:B:282:MET:HG2	2:B:296:VAL:HG13	1.99	0.44
2:B:213:LEU:HD23	2:B:412:THR:HG22	2.00	0.44
1:A:204:GLN:HA	2:B:245:MET:SD	2.58	0.44
1:A:166:TYR:HE1	5:B:1001:FTH:H232	1.82	0.44
1:A:239:GLN:O	1:A:243:VAL:HG23	2.18	0.44
2:B:420:VAL:O	2:B:422:GLY:N	2.50	0.44
2:B:248:HIS:CE1	4:B:501:HFP:H62	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:58:LEU:O	1:A:95:LYS:NZ	2.49	0.44
1:A:112:ARG:O	1:A:144:LEU:HD21	2.18	0.44
2:B:331:HIS:CD2	2:B:334:ALA:H	2.36	0.44
2:B:194:HIS:CD2	2:B:197:GLY:HA3	2.53	0.44
1:A:72:TRP:CZ3	1:A:75:ILE:HD12	2.53	0.43
2:B:173:ASN:CG	2:B:176:LYS:HB2	2.39	0.43
1:A:77:PRO:HB2	1:A:101:ASP:HB3	2.00	0.43
1:A:319:TYR:CE1	1:A:336:LYS:HG3	2.53	0.43
2:B:303:TRP:CH2	4:B:501:HFP:H121	2.53	0.43
1:A:316:VAL:O	1:A:320:GLU:HG3	2.17	0.43
2:B:237:GLY:O	2:B:273:LEU:HA	2.19	0.43
4:B:501:HFP:H112	5:B:1001:FTH:HC28	2.00	0.43
1:A:339:GLU:O	1:A:343:ILE:HG13	2.18	0.43
2:B:46:ILE:O	2:B:50:LYS:HG3	2.18	0.43
2:B:398:HIS:HD2	2:B:408:VAL:HG11	1.83	0.43
2:B:376:PHE:CG	2:B:377:GLY:N	2.86	0.43
2:B:149:HIS:HB3	2:B:152:PRO:HD2	1.99	0.43
2:B:122:VAL:HG13	2:B:123:ALA:N	2.33	0.43
2:B:99:SER:O	2:B:102:TRP:HB2	2.19	0.43
2:B:163:ILE:HG22	2:B:165:THR:HG23	2.00	0.43
4:B:501:HFP:H52	5:B:1001:FTH:C23	2.49	0.43
1:A:260:VAL:HG21	1:A:284:LEU:HD21	2.00	0.43
2:B:24:TYR:HB2	2:B:333:GLN:CD	2.39	0.43
2:B:175:GLU:H	2:B:175:GLU:CD	2.22	0.43
1:A:99:VAL:HG13	1:A:119:LEU:CD1	2.49	0.43
1:A:227:LEU:HD23	1:A:227:LEU:HA	1.91	0.42
2:B:121:ILE:HD12	2:B:121:ILE:H	1.83	0.42
1:A:155:ILE:HD12	1:A:155:ILE:HA	1.88	0.42
1:A:312:ILE:HB	1:A:344:LEU:HD21	2.02	0.42
2:B:409:ILE:O	2:B:413:THR:HG23	2.19	0.42
2:B:204:ALA:HB1	2:B:229:ILE:HD11	2.01	0.42
2:B:403:ILE:HG13	2:B:408:VAL:HG23	2.00	0.42
2:B:408:VAL:O	2:B:412:THR:HG23	2.20	0.42
2:B:331:HIS:HD2	2:B:334:ALA:H	1.66	0.42
1:A:232:ARG:NH1	2:B:42:THR:HG23	2.34	0.42
2:B:29:GLU:O	2:B:32:ARG:HD2	2.20	0.42
4:B:501:HFP:H21	5:B:1001:FTH:H231	2.01	0.42
2:B:238:GLY:HA3	2:B:247:ALA:HB1	2.01	0.42
2:B:173:ASN:OD1	2:B:175:GLU:HG2	2.19	0.42
2:B:333:GLN:HG3	2:B:387:MET:CE	2.49	0.42
2:B:291:ARG:HB2	2:B:294:LYS:CG	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:218:THR:CB	2:B:219:PRO:HD2	2.44	0.42
1:A:112:ARG:HA	1:A:140:LEU:HD21	2.02	0.42
1:A:322:MET:HE3	1:A:333:ILE:CD1	2.43	0.41
2:B:335:LEU:HD23	2:B:373:ALA:HB2	2.02	0.41
1:A:103:PHE:HE1	1:A:120:THR:HG22	1.85	0.41
1:A:99:VAL:HG13	1:A:119:LEU:HD11	2.02	0.41
4:B:501:HFP:H112	5:B:1001:FTH:C29	2.50	0.41
1:A:287:ARG:CD	1:A:291:ARG:HD3	2.45	0.41
2:B:294:LYS:HA	2:B:294:LYS:HD2	1.94	0.41
1:A:272:HIS:CD2	1:A:308:SER:HB3	2.56	0.41
1:A:57:SER:O	1:A:63:TYR:HD1	2.04	0.41
2:B:320:ASP:HA	2:B:321:PRO:HD3	1.70	0.41
4:B:501:HFP:H61	5:B:1001:FTH:H231	2.02	0.41
1:A:302:LEU:HB3	1:A:306:HIS:HB2	2.02	0.41
1:A:338:LEU:HD21	1:A:363:LEU:HB3	2.01	0.41
2:B:211:ALA:HA	2:B:216:ILE:CG1	2.51	0.41
2:B:213:LEU:HG	2:B:401:TYR:CE2	2.56	0.41
2:B:122:VAL:CG1	2:B:123:ALA:N	2.84	0.41
1:A:58:LEU:HD22	1:A:95:LYS:HE3	2.02	0.41
1:A:65:LEU:O	1:A:69:ARG:HG3	2.21	0.41
1:A:207:GLN:O	1:A:211:GLN:HB2	2.21	0.40
1:A:363:LEU:HA	1:A:363:LEU:HD12	1.90	0.40
2:B:403:ILE:HG13	2:B:408:VAL:CG2	2.52	0.40
1:A:72:TRP:CZ2	1:A:115:ARG:HD2	2.57	0.40
1:A:328:ASP:O	1:A:329:ASN:CB	2.68	0.40
1:A:66:TYR:CZ	1:A:119:LEU:HD13	2.55	0.40
1:A:323:LEU:HD13	1:A:333:ILE:HG21	2.02	0.40
2:B:27:ARG:HA	2:B:28:PRO:HD3	1.87	0.40
2:B:34:ARG:HD2	2:B:284:PHE:CE1	2.56	0.40

All (3) 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:60:SER:OG	1:A:257:GLU:OE1[6_555]	2.08	0.12
1:A:251:SER:CB	2:B:120:GLN:OE1[2_655]	2.17	0.03
1:A:74:ASP:O	2:B:84:ARG:NH2[4_665]	2.19	0.01

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	310/315 (98%)	278 (90%)	27 (9%)	5 (2%)	12	11
2	B	399/402 (99%)	370 (93%)	26 (6%)	3 (1%)	24	27
All	All	709/717 (99%)	648 (91%)	53 (8%)	8 (1%)	17	18

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	287	ARG
2	B	74	GLN
1	A	326	GLN
2	B	378	SER
1	A	197	ALA
2	B	421	PRO
1	A	88	VAL
1	A	304	PRO

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	291/294 (99%)	270 (93%)	21 (7%)	18	22
2	B	338/339 (100%)	321 (95%)	17 (5%)	30	41
All	All	629/633 (99%)	591 (94%)	38 (6%)	24	31

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	56	LEU
1	A	87	VAL
1	A	121	ARG
1	A	162	GLN
1	A	214	ARG
1	A	221	GLN
1	A	251	SER
1	A	265	GLU
1	A	269	LEU
1	A	286	ASP
1	A	289	LEU
1	A	298	GLN
1	A	300	LEU
1	A	323	LEU
1	A	330	LYS
1	A	339	GLU
1	A	342	GLU
1	A	348	LYS
1	A	352	ARG
1	A	363	LEU
1	A	366	LYS
2	B	29	GLU
2	B	45	SER
2	B	68	VAL
2	B	70	ARG
2	B	77	LYS
2	B	84	ARG
2	B	201	VAL
2	B	245	MET
2	B	266	ARG
2	B	271	LYS
2	B	275	GLN
2	B	296	VAL
2	B	332	GLN
2	B	351	LEU
2	B	382	LEU
2	B	387	MET
2	B	423	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	80	GLN

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Mol	Chain	Res	Type
1	A	149	GLN
1	A	184	GLN
1	A	201	HIS
1	A	204	GLN
1	A	221	GLN
1	A	246	ASN
1	A	261	GLN
1	A	285	GLN
1	A	306	HIS
1	A	325	ASN
1	A	364	GLN
2	B	48	GLN
2	B	146	GLN
2	B	275	GLN
2	B	331	HIS
2	B	332	GLN
2	B	392	ASN

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](#)

Of 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 for Mogul analysis.

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
5	FTH	B	1001	3	40,42,42	1.85	12 (30%)	46,58,58	1.60	6 (13%)
4	HFP	B	501	-	16,19,19	1.58	2 (12%)	20,25,25	1.57	4 (20%)

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
5	FTH	B	1001	3	-	0/23/38/38	0/5/5/5
4	HFP	B	501	-	2/2/5/5	0/20/22/22	0/0/0/0

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	501	HFP	C2-C3	-4.19	1.35	1.53
5	B	1001	FTH	C22-N21	-3.80	1.40	1.47
4	B	501	HFP	C7-C8	-3.14	1.36	1.52
5	B	1001	FTH	C22-C23	-2.24	1.48	1.52
5	B	1001	FTH	C34-C35	2.07	1.41	1.36
5	B	1001	FTH	C18-C11	2.21	1.43	1.38
5	B	1001	FTH	C18-C17	2.27	1.42	1.38
5	B	1001	FTH	C8-C19	2.44	1.58	1.53
5	B	1001	FTH	C33-C32	2.63	1.42	1.36
5	B	1001	FTH	C13-C12	2.69	1.43	1.38
5	B	1001	FTH	C7-C6	3.09	1.55	1.50
5	B	1001	FTH	C26-N21	3.19	1.51	1.46
5	B	1001	FTH	C37-C24	3.53	1.46	1.43
5	B	1001	FTH	C28-C27	3.61	1.44	1.37

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	1001	FTH	C24-C37-N38	-2.93	171.88	177.11
4	B	501	HFP	O1P-P-C1	-2.44	107.29	112.66
5	B	1001	FTH	C10-N9-C8	2.01	116.88	113.81
4	B	501	HFP	C2-C3-C5	2.53	122.14	112.38
4	B	501	HFP	C9-C8-C7	2.61	121.11	111.08
5	B	1001	FTH	C1-N2-C6	2.78	128.14	124.44
4	B	501	HFP	C4-C3-C2	3.06	121.84	110.92
5	B	1001	FTH	C26-N21-C22	3.17	122.15	114.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	1001	FTH	C23-C22-N21	3.44	116.43	110.50
5	B	1001	FTH	C22-C23-C24	6.71	118.40	109.08

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	B	501	HFP	C3
4	B	501	HFP	C8

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	1001	FTH	14	0
4	B	501	HFP	10	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th 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 ²)	Q<0.9
1	A	312/315 (99%)	1.76	104 (33%) 0 0	13, 41, 82, 100	0
2	B	401/402 (99%)	1.41	96 (23%) 1 1	11, 35, 72, 100	0
All	All	713/717 (99%)	1.56	200 (28%) 1 1	11, 37, 78, 100	0

All (200) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	117	PRO	13.1
1	A	55	PHE	12.8
2	B	423	PHE	12.1
1	A	56	LEU	9.7
1	A	61	PRO	7.6
2	B	40	VAL	7.4
1	A	326	GLN	7.4
2	B	122	VAL	7.4
2	B	378	SER	6.3
1	A	62	THR	6.1
1	A	306	HIS	6.1
2	B	422	GLY	6.1
1	A	291	ARG	5.8
2	B	84	ARG	5.7
2	B	87	ARG	5.3
1	A	366	LYS	5.3
2	B	80	HIS	5.2
2	B	128	GLN	5.1
1	A	87	VAL	4.9
1	A	58	LEU	4.9
1	A	57	SER	4.7
2	B	132	LEU	4.6
1	A	149	GLN	4.6
1	A	182	PRO	4.4

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Mol	Chain	Res	Type	RSRZ
1	A	186	LEU	4.4
2	B	195	VAL	4.3
1	A	70	ALA	4.3
2	B	64	PHE	4.2
2	B	382	LEU	4.2
1	A	299	LEU	4.2
1	A	214	ARG	4.1
1	A	216	TRP	4.1
2	B	92	ALA	4.1
1	A	288	GLY	4.1
2	B	119	PRO	4.1
1	A	184	GLN	4.0
1	A	255	VAL	4.0
1	A	152	MET	4.0
2	B	179	GLN	3.8
1	A	221	GLN	3.8
2	B	409	ILE	3.8
1	A	323	LEU	3.7
2	B	322	ALA	3.7
1	A	292	TYR	3.7
1	A	295	LEU	3.7
1	A	225	GLN	3.6
2	B	76	GLU	3.6
1	A	303	GLN	3.6
1	A	63	TYR	3.6
2	B	221	LEU	3.6
2	B	83	LYS	3.5
2	B	389	VAL	3.5
1	A	217	ASP	3.5
1	A	180	LYS	3.4
1	A	64	VAL	3.4
1	A	174	VAL	3.4
1	A	173	ARG	3.4
1	A	145	GLN	3.4
2	B	120	GLN	3.4
2	B	211	ALA	3.4
2	B	171	VAL	3.4
1	A	215	LEU	3.4
1	A	65	LEU	3.3
1	A	363	LEU	3.3
2	B	129	PHE	3.3
1	A	335	ASN	3.3

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Mol	Chain	Res	Type	RSRZ
2	B	113	LEU	3.3
1	A	286	ASP	3.2
2	B	266	ARG	3.2
2	B	163	ILE	3.2
2	B	180	TYR	3.2
2	B	104	CYS	3.2
2	B	124	THR	3.2
1	A	60	SER	3.2
1	A	142	ARG	3.2
2	B	121	ILE	3.1
1	A	260	VAL	3.1
2	B	377	GLY	3.1
1	A	89	GLN	3.1
2	B	417	GLN	3.1
2	B	115	ASP	3.1
1	A	348	LYS	3.1
2	B	43	VAL	3.1
1	A	86	PRO	3.1
1	A	324	GLU	3.0
2	B	199	VAL	3.0
1	A	307	SER	3.0
2	B	394	LEU	3.0
2	B	210	VAL	3.0
1	A	302	LEU	3.0
1	A	333	ILE	3.0
2	B	181	LEU	3.0
1	A	277	TRP	3.0
1	A	293	PRO	2.9
2	B	28	PRO	2.9
2	B	118	ILE	2.9
2	B	99	SER	2.9
1	A	264	LEU	2.9
1	A	195	GLN	2.9
1	A	327	CYS	2.9
1	A	271	PRO	2.9
2	B	32	ARG	2.9
1	A	224	ASP	2.9
1	A	322	MET	2.9
2	B	139	GLY	2.9
2	B	381	MET	2.9
1	A	268	LYS	2.9
2	B	225	THR	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	72	TRP	2.8
2	B	125	ASP	2.8
2	B	111	LEU	2.8
1	A	242	PHE	2.8
1	A	305	SER	2.8
2	B	126	VAL	2.7
2	B	383	HIS	2.7
2	B	392	ASN	2.7
1	A	178	TRP	2.7
2	B	36	GLN	2.7
1	A	218	ASN	2.7
1	A	276	ALA	2.7
1	A	346	LYS	2.7
2	B	170	ASN	2.6
1	A	265	GLU	2.6
2	B	166	GLU	2.6
2	B	194	HIS	2.6
1	A	190	ALA	2.6
2	B	35	LEU	2.6
1	A	329	ASN	2.6
2	B	240	GLY	2.5
2	B	168	ALA	2.5
2	B	95	CYS	2.5
1	A	269	LEU	2.5
1	A	88	VAL	2.5
1	A	236	VAL	2.5
1	A	201	HIS	2.5
1	A	310	TYR	2.5
2	B	62	TYR	2.5
1	A	95	LYS	2.5
2	B	418	LYS	2.5
1	A	211	GLN	2.5
2	B	37	ASP	2.5
2	B	42	THR	2.4
1	A	330	LYS	2.4
1	A	84	PRO	2.4
1	A	272	HIS	2.4
2	B	108	LEU	2.4
2	B	176	LYS	2.4
1	A	97	ARG	2.4
2	B	82	LEU	2.4
1	A	68	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	287	ARG	2.4
1	A	228	LYS	2.3
1	A	237	TRP	2.3
1	A	362	SER	2.3
1	A	158	ILE	2.3
1	A	220	LEU	2.3
1	A	256	LEU	2.3
2	B	214	THR	2.3
1	A	318	ILE	2.3
2	B	319	GLY	2.3
2	B	311	LEU	2.3
2	B	380	ALA	2.3
2	B	160	LEU	2.3
2	B	156	ALA	2.2
2	B	217	ILE	2.2
2	B	223	GLU	2.2
2	B	333	GLN	2.2
2	B	411	ALA	2.2
1	A	223	VAL	2.2
1	A	187	GLU	2.2
2	B	313	ARG	2.2
2	B	413	THR	2.2
1	A	125	GLU	2.2
1	A	166	TYR	2.2
2	B	169	TYR	2.2
1	A	230	ASP	2.2
1	A	144	LEU	2.2
2	B	172	ILE	2.2
2	B	157	VAL	2.2
2	B	85	GLY	2.2
2	B	284	PHE	2.2
1	A	219	GLU	2.2
2	B	178	LEU	2.2
1	A	209	VAL	2.1
2	B	177	LEU	2.1
1	A	121	ARG	2.1
1	A	252	ASP	2.1
2	B	373	ALA	2.1
2	B	107	ILE	2.1
2	B	183	SER	2.1
1	A	109	ARG	2.1
2	B	67	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
2	B	127	CYS	2.1
1	A	59	ASP	2.1
2	B	149	HIS	2.1
2	B	162	ILE	2.1
1	A	226	LEU	2.0
2	B	97	ASP	2.0
1	A	259	GLU	2.0
1	A	312	ILE	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th 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(\AA^2)	Q<0.9
4	HFP	B	501	20/20	0.76	0.31	2.89	30,30,30,30	0
5	FTH	B	1001	38/38	0.82	0.28	1.83	30,30,30,30	0
3	ZN	B	500	1/1	0.98	0.17	0.22	30,30,30,30	0

6.5 Other polymers [i](#)

There are no such residues in this entry.