Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 11:46 AM GMT

PDB ID	:	3PZ4
Title	:	Crystal structure of FTase(ALPHA-subunit; BETA-subunit DELTA C10) in complex with BMS3 and lipid substrate FPP
Authors	:	Guo, Z.; Bon, R.S.; Stigter, E.A.; Waldmann, H.; Alexandrov, K.; Blankenfeldt, W.; Goody, R.S.
Deposited on	:	2010-12-14
Resolution	:	2.10 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
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

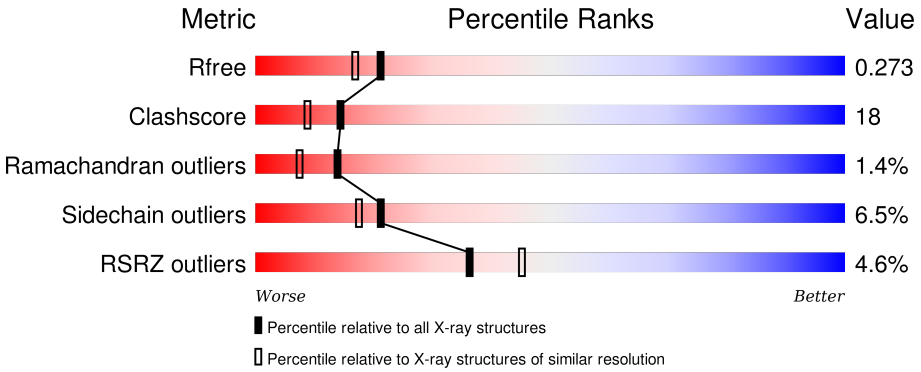
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	3939 (2.10-2.10)
Clashscore	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)
RSRZ outliers	91569	3948 (2.10-2.10)

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 <=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	379	5%, 50%, 28%, 17%
2	B	426	3%, 65%, 26%, 5%

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	FPP	B	428	-	-	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 6208 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/geranylgeranyltransferase type-1 subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	315	2670	1703	470	492	5	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	EXPRESSION TAG	UNP Q04631
A	0	HIS	-	EXPRESSION TAG	UNP Q04631

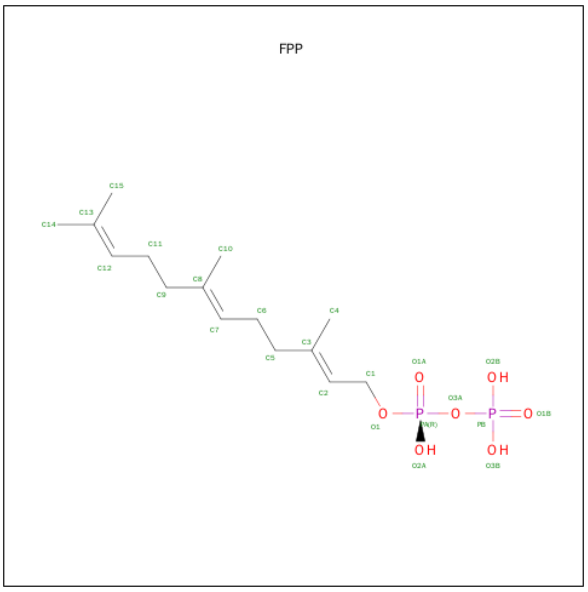
- Molecule 2 is a protein called Protein farnesyltransferase subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	403	3169	2026	545	575	23	0	0	0

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

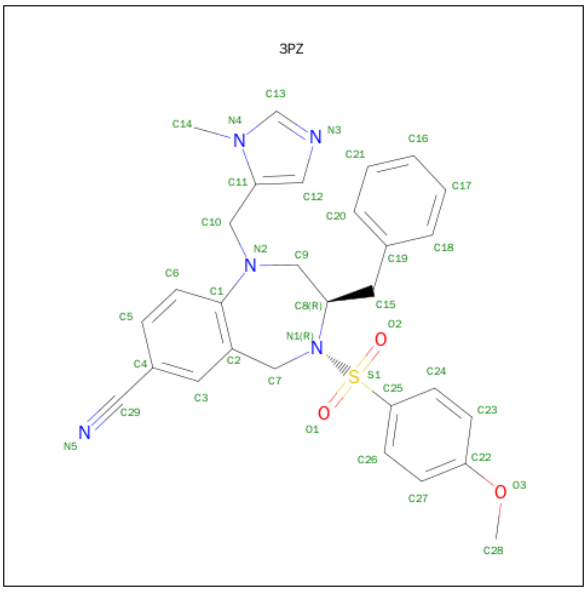
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
3	B	1	1	1	0	0

- Molecule 4 is FARNESYL DIPHOSPHATE (three-letter code: FPP) (formula: $C_{15}H_{28}O_7P_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	P		
4	B	1	24	15	7	2	0	0

- Molecule 5 is (3R)-3-BENZYL-4-[(4-METHOXYPHENYL)SULFONYL]-1-[(1-METHYL-1 H-IMIDAZOL-5-YL)METHYL]-2,3,4,5-TETRAHYDRO-1H-1,4-BENZODIAZEPINE-7-C ARBONITRILE (three-letter code: 3PZ) (formula: $C_{29}H_{29}N_5O_3S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
5	B	1	38	29	5	3	1	0	0

- Molecule 6 is water.

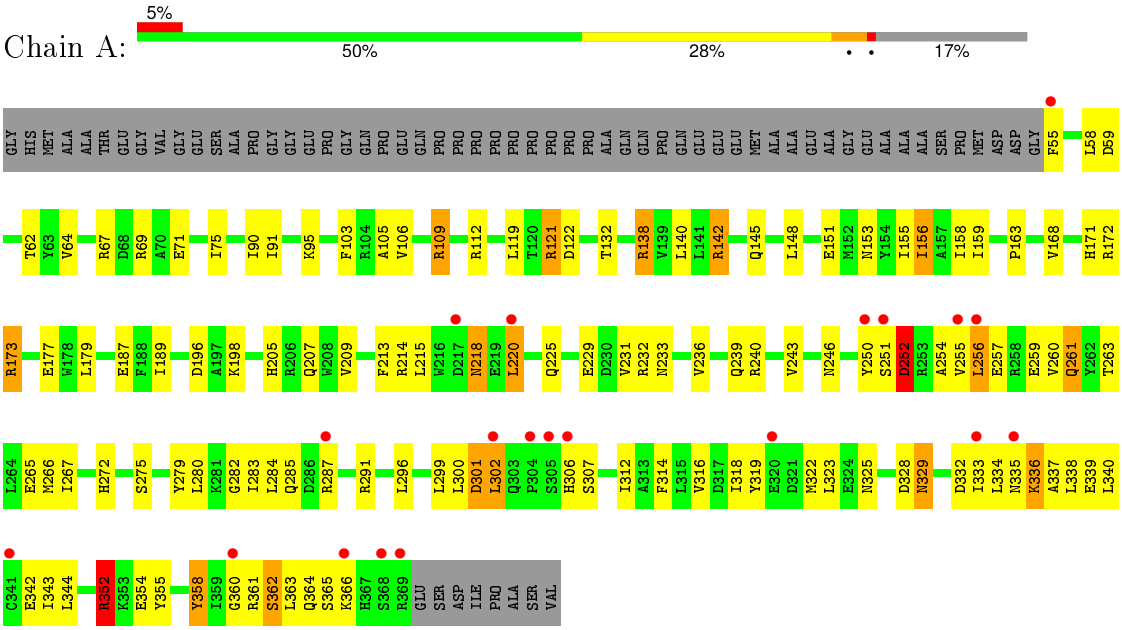
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	137	Total O 137 137	0	0
6	B	169	Total O 169 169	0	0

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.

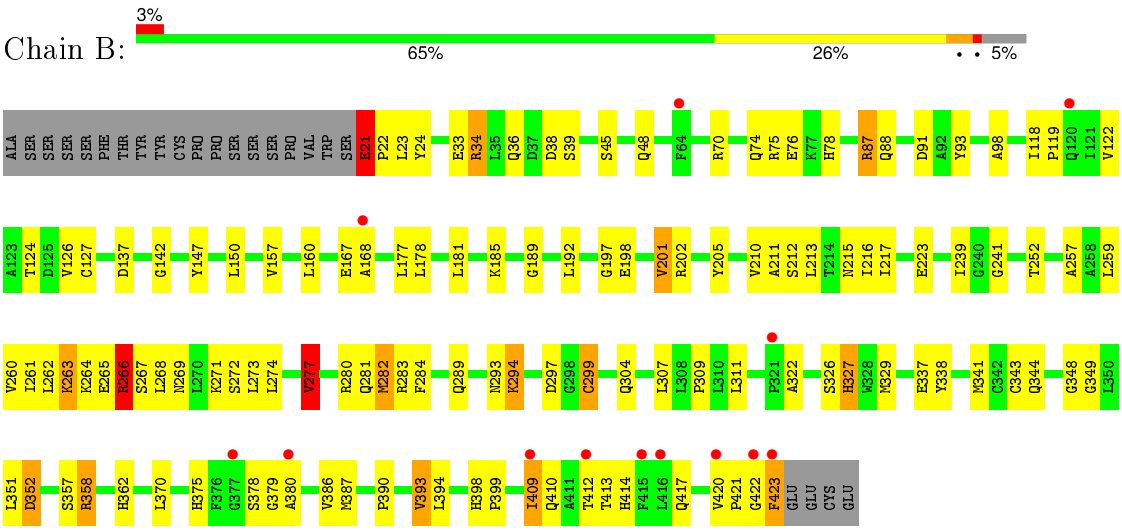
- Molecule 1: Protein farnesyltransferase/geranylgeranyltransferase type-1 subunit alpha

Chain A:



- Molecule 2: Protein farnesyltransferase subunit beta

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α, β, γ	170.75Å 170.75Å 69.08Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.91 – 2.10 29.57 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.8 (29.91-2.10) 99.8 (29.57-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$< I/\sigma(I) >$ [1]	5.90 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.225 , 0.267 0.233 , 0.273	Depositor DCC
R_{free} test set	3365 reflections (5.28%)	DCC
Wilson B-factor (Å^2)	26.4	Xtriage
Anisotropy	0.385	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 30.9	EDS
Estimated twinning fraction	0.094 for h,-h-k,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.39$, $< L^2 > = 0.22$	Xtriage
Outliers	0 of 67102 reflections	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	6208	wwPDB-VP
Average B, all atoms (Å^2)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.94% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: 3PZ, ZN, FPP

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	0.81	0/2736	0.86	9/3716 (0.2%)
2	B	0.80	1/3255 (0.0%)	0.83	7/4421 (0.2%)
All	All	0.80	1/5991 (0.0%)	0.84	16/8137 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
2	B	1	1
All	All	1	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	299	CYS	CB-SG	-6.47	1.71	1.82

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	138	ARG	NE-CZ-NH2	-8.74	115.93	120.30
1	A	173	ARG	NE-CZ-NH1	7.87	124.23	120.30
1	A	142	ARG	NE-CZ-NH2	7.66	124.13	120.30
1	A	138	ARG	NE-CZ-NH1	6.03	123.31	120.30
2	B	21	GLU	N-CA-C	5.96	127.10	111.00
2	B	358	ARG	CB-CA-C	-5.88	98.64	110.40
2	B	297	ASP	CB-CG-OD1	5.62	123.36	118.30
1	A	142	ARG	NE-CZ-NH1	-5.59	117.50	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	122	ASP	CB-CG-OD1	5.53	123.27	118.30
2	B	352	ASP	CB-CG-OD1	5.39	123.15	118.30
1	A	220	LEU	CA-CB-CG	5.35	127.60	115.30
2	B	277	VAL	CB-CA-C	-5.32	101.30	111.40
2	B	282	MET	CG-SD-CE	5.29	108.66	100.20
1	A	196	ASP	CB-CG-OD1	5.17	122.95	118.30
1	A	352	ARG	NE-CZ-NH2	-5.10	117.75	120.30
2	B	201	VAL	CB-CA-C	-5.06	101.78	111.40

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	B	21	GLU	CA

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	251	SER	Peptide
2	B	21	GLU	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2670	0	2587	111	0
2	B	3169	0	3098	111	1
3	B	1	0	0	0	0
4	B	24	0	25	2	0
5	B	38	0	29	0	0
6	A	137	0	0	32	5
6	B	169	0	0	20	6
All	All	6208	0	5739	210	7

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 (210) 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:355:TYR:HA	6:A:509:HOH:O	1.48	1.09
2:B:33:GLU:OE1	6:B:581:HOH:O	1.79	1.01
6:A:509:HOH:O	2:B:329:MET:SD	2.19	0.98
1:A:296:LEU:HD22	1:A:322:MET:CE	1.97	0.94
2:B:266:ARG:HA	6:B:582:HOH:O	1.68	0.92
1:A:340:LEU:HA	6:A:481:HOH:O	1.68	0.92
2:B:78:HIS:HD1	2:B:349:GLY:H	1.13	0.90
1:A:272:HIS:ND1	6:A:511:HOH:O	2.04	0.87
2:B:280:ARG:NH1	2:B:289:GLN:HE21	1.72	0.87
2:B:262:LEU:O	2:B:263:LYS:HB2	1.75	0.85
2:B:280:ARG:NH1	2:B:289:GLN:NE2	2.26	0.83
1:A:209:VAL:HG13	6:A:498:HOH:O	1.81	0.81
1:A:296:LEU:HD22	1:A:322:MET:HE1	1.61	0.80
1:A:338:LEU:CD2	1:A:360:GLY:O	2.28	0.80
2:B:74:GLN:H	2:B:344:GLN:HE22	1.30	0.78
2:B:87:ARG:HD3	6:B:543:HOH:O	1.82	0.78
1:A:58:LEU:HD22	1:A:95:LYS:HD3	1.64	0.78
2:B:76:GLU:HB3	6:B:552:HOH:O	1.82	0.77
2:B:22:PRO:HD2	6:B:541:HOH:O	1.83	0.77
1:A:296:LEU:HD22	1:A:322:MET:HE3	1.65	0.77
2:B:23:LEU:HD23	6:B:555:HOH:O	1.86	0.76
1:A:339:GLU:HG2	6:A:481:HOH:O	1.85	0.75
1:A:142:ARG:HD2	6:A:383:HOH:O	1.85	0.75
1:A:338:LEU:HD21	1:A:360:GLY:O	1.87	0.74
1:A:254:ALA:O	6:A:480:HOH:O	2.06	0.73
2:B:387:MET:CE	6:B:555:HOH:O	2.38	0.71
1:A:207:GLN:HE21	1:A:239:GLN:HE22	1.36	0.71
2:B:386:VAL:HG21	2:B:393:VAL:CG1	2.20	0.71
1:A:265:GLU:HB2	6:A:471:HOH:O	1.88	0.71
1:A:255:VAL:C	1:A:257:GLU:H	1.94	0.71
1:A:301:ASP:HB3	1:A:302:LEU:HD23	1.73	0.71
2:B:280:ARG:HH11	2:B:289:GLN:HE21	1.38	0.69
1:A:343:ILE:HG13	6:A:481:HOH:O	1.93	0.68
1:A:148:LEU:HB2	1:A:179:LEU:HD21	1.75	0.68
2:B:157:VAL:HG21	2:B:210:VAL:HG13	1.74	0.67
1:A:69:ARG:O	6:A:404:HOH:O	2.13	0.67
1:A:255:VAL:O	1:A:257:GLU:N	2.25	0.66
1:A:156:ILE:HG12	1:A:172:ARG:HH12	1.60	0.66
2:B:280:ARG:HH11	2:B:289:GLN:NE2	1.93	0.66
2:B:33:GLU:HG2	6:B:590:HOH:O	1.96	0.66
2:B:386:VAL:HG21	2:B:393:VAL:HG13	1.79	0.65
2:B:259:LEU:HD22	2:B:264:LYS:HB2	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:243:VAL:O	1:A:246:ASN:N	2.24	0.65
1:A:213:PHE:CD1	6:A:498:HOH:O	2.49	0.65
1:A:361:ARG:HG2	2:B:322:ALA:HB1	1.80	0.64
1:A:218:ASN:HD22	1:A:218:ASN:N	1.97	0.63
2:B:217:ILE:HB	6:B:592:HOH:O	1.97	0.63
2:B:78:HIS:HD1	2:B:349:GLY:N	1.92	0.63
2:B:215:ASN:O	2:B:420:VAL:HG22	1.97	0.63
1:A:173:ARG:O	1:A:177:GLU:HG2	1.99	0.62
1:A:62:THR:O	1:A:64:VAL:HG23	2.00	0.62
1:A:328:ASP:O	1:A:329:ASN:CB	2.47	0.62
1:A:173:ARG:HD3	6:B:514:HOH:O	1.99	0.62
2:B:178:LEU:HD23	2:B:421:PRO:O	2.00	0.61
2:B:259:LEU:HD12	2:B:268:LEU:HD11	1.82	0.61
2:B:177:LEU:HD21	2:B:210:VAL:CG1	2.31	0.61
1:A:318:ILE:CG2	1:A:322:MET:HE2	2.32	0.60
2:B:211:ALA:HB1	2:B:217:ILE:HG12	1.83	0.60
1:A:299:LEU:HD11	1:A:314:PHE:HD2	1.66	0.60
1:A:319:TYR:O	1:A:323:LEU:HD12	2.02	0.60
1:A:207:GLN:HE21	1:A:239:GLN:NE2	2.00	0.59
1:A:299:LEU:HD11	1:A:314:PHE:CD2	2.36	0.59
2:B:118:ILE:HG22	2:B:122:VAL:CG2	2.32	0.59
1:A:275:SER:OG	2:B:293:ASN:ND2	2.35	0.59
2:B:74:GLN:H	2:B:344:GLN:NE2	1.99	0.59
1:A:291:ARG:HD2	6:A:496:HOH:O	2.02	0.58
1:A:336:LYS:NZ	1:A:336:LYS:HB3	2.19	0.58
2:B:118:ILE:CG2	2:B:122:VAL:CG2	2.82	0.57
1:A:158:ILE:N	1:A:158:ILE:HD13	2.18	0.57
1:A:318:ILE:CG2	1:A:322:MET:CE	2.82	0.57
1:A:322:MET:O	1:A:325:ASN:O	2.23	0.57
1:A:256:LEU:HG	1:A:256:LEU:O	2.03	0.57
2:B:272:SER:HA	6:B:569:HOH:O	2.04	0.57
2:B:272:SER:CA	6:B:569:HOH:O	2.53	0.57
1:A:334:LEU:HD22	6:A:482:HOH:O	2.03	0.57
1:A:255:VAL:C	1:A:257:GLU:N	2.58	0.56
2:B:223:GLU:HG3	6:B:572:HOH:O	2.04	0.56
2:B:378:SER:O	2:B:380:ALA:N	2.38	0.56
1:A:283:ILE:C	6:A:507:HOH:O	2.44	0.56
1:A:109:ARG:NH1	6:A:443:HOH:O	2.39	0.56
1:A:329:ASN:CB	1:A:332:ASP:HB3	2.37	0.55
1:A:302:LEU:HB3	1:A:306:HIS:HB2	1.88	0.55
1:A:261:GLN:O	6:A:471:HOH:O	2.18	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:267:ILE:O	1:A:267:ILE:HG22	2.07	0.54
2:B:124:THR:HG23	2:B:167:GLU:OE2	2.08	0.54
2:B:264:LYS:O	2:B:265:GLU:C	2.46	0.54
2:B:259:LEU:O	2:B:263:LYS:N	2.38	0.53
2:B:177:LEU:HD21	2:B:210:VAL:HG12	1.89	0.53
1:A:260:VAL:CG2	1:A:284:LEU:HD21	2.38	0.53
1:A:121:ARG:CD	6:A:500:HOH:O	2.55	0.53
1:A:299:LEU:CD1	1:A:314:PHE:HD2	2.21	0.53
1:A:155:ILE:HD13	1:A:171:HIS:CD2	2.44	0.53
1:A:343:ILE:CG1	6:A:481:HOH:O	2.54	0.53
1:A:159:ILE:HG12	1:A:168:VAL:HG13	1.91	0.52
1:A:187:GLU:HB2	6:A:489:HOH:O	2.08	0.52
2:B:264:LYS:O	2:B:266:ARG:N	2.43	0.52
1:A:231:VAL:HG21	1:A:266:MET:HE2	1.92	0.52
1:A:352:ARG:NH2	2:B:281:GLN:O	2.43	0.52
2:B:280:ARG:HH12	2:B:289:GLN:NE2	2.07	0.52
2:B:387:MET:HE1	6:B:555:HOH:O	2.05	0.52
2:B:202:ARG:HD2	4:B:428:FPP:H142	1.91	0.52
1:A:355:TYR:HD1	6:A:509:HOH:O	1.93	0.52
1:A:279:TYR:O	1:A:282:GLY:N	2.43	0.52
2:B:150:LEU:HD21	2:B:181:LEU:CD2	2.39	0.52
2:B:239:ILE:HB	2:B:252:THR:HA	1.92	0.52
2:B:375:HIS:HE1	2:B:394:LEU:O	1.93	0.52
1:A:282:GLY:HA2	1:A:285:GLN:NE2	2.25	0.52
1:A:225:GLN:O	1:A:229:GLU:HG3	2.10	0.52
2:B:386:VAL:CG2	2:B:393:VAL:CG1	2.87	0.51
1:A:62:THR:O	1:A:62:THR:HG22	2.09	0.51
1:A:302:LEU:N	1:A:302:LEU:HD23	2.26	0.51
1:A:363:LEU:HD23	1:A:366:LYS:HE2	1.93	0.51
2:B:272:SER:CB	6:B:569:HOH:O	2.59	0.51
2:B:201:VAL:HG23	2:B:241:GLY:O	2.11	0.50
1:A:312:ILE:HG23	1:A:340:LEU:HD22	1.93	0.50
2:B:98:ALA:O	2:B:142:GLY:HA3	2.11	0.50
2:B:338:TYR:CE2	2:B:343:CYS:SG	3.04	0.50
1:A:103:PHE:HA	1:A:119:LEU:HD21	1.91	0.50
1:A:272:HIS:CE1	6:A:511:HOH:O	2.58	0.50
1:A:250:TYR:OH	1:A:279:TYR:OH	2.17	0.50
1:A:232:ARG:NH1	2:B:45:SER:HB3	2.27	0.50
2:B:118:ILE:CG2	2:B:122:VAL:HG23	2.42	0.49
1:A:257:GLU:O	1:A:261:GLN:HB2	2.11	0.49
1:A:338:LEU:HD22	1:A:360:GLY:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:390:PRO:O	2:B:393:VAL:HG22	2.13	0.49
2:B:24:TYR:OH	6:B:581:HOH:O	2.20	0.49
6:A:511:HOH:O	2:B:36:GLN:HB3	2.13	0.49
1:A:218:ASN:N	1:A:218:ASN:ND2	2.60	0.49
2:B:257:ALA:O	2:B:261:ILE:HG13	2.14	0.48
2:B:423:PHE:CD2	2:B:423:PHE:C	2.87	0.48
1:A:318:ILE:HG22	1:A:322:MET:CE	2.44	0.48
2:B:185:LYS:HZ3	2:B:189:GLY:C	2.17	0.48
1:A:213:PHE:HB2	1:A:215:LEU:HD12	1.96	0.48
1:A:361:ARG:HG2	2:B:322:ALA:CB	2.44	0.48
1:A:263:THR:HG21	1:A:280:LEU:HB2	1.97	0.47
1:A:173:ARG:NH1	2:B:198:GLU:OE2	2.44	0.47
2:B:378:SER:N	6:B:597:HOH:O	2.48	0.47
2:B:192:LEU:HD22	2:B:197:GLY:O	2.15	0.47
6:A:509:HOH:O	2:B:329:MET:CG	2.57	0.47
2:B:75:ARG:NH2	2:B:393:VAL:O	2.48	0.47
2:B:280:ARG:HG3	2:B:304:GLN:NE2	2.30	0.46
2:B:264:LYS:C	2:B:266:ARG:N	2.65	0.46
1:A:90:ILE:HD13	2:B:93:TYR:O	2.15	0.46
1:A:233:ASN:CG	1:A:236:VAL:HG23	2.35	0.46
2:B:414:HIS:O	2:B:417:GLN:HB2	2.15	0.46
2:B:277:VAL:HG13	2:B:307:LEU:HD12	1.96	0.46
2:B:387:MET:HE3	6:B:555:HOH:O	2.07	0.46
1:A:106:VAL:HG21	1:A:119:LEU:HD23	1.97	0.46
2:B:370:LEU:HD23	2:B:394:LEU:HD11	1.98	0.46
1:A:91:ILE:O	2:B:91:ASP:HB3	2.15	0.46
2:B:272:SER:HB2	6:B:569:HOH:O	2.15	0.45
1:A:105:ALA:O	1:A:109:ARG:HG3	2.17	0.45
1:A:252:ASP:OD1	1:A:254:ALA:N	2.49	0.45
2:B:216:ILE:HG22	2:B:421:PRO:HD2	1.99	0.45
1:A:198:LYS:CD	2:B:294:LYS:HD3	2.46	0.45
2:B:259:LEU:HD12	2:B:268:LEU:CD1	2.46	0.45
1:A:231:VAL:HG21	1:A:266:MET:CE	2.47	0.44
2:B:409:ILE:HG22	2:B:410:GLN:N	2.33	0.44
2:B:273:LEU:O	2:B:274:LEU:C	2.55	0.44
1:A:240:ARG:HD3	1:A:259:GLU:OE1	2.18	0.44
1:A:284:LEU:N	6:A:507:HOH:O	2.49	0.44
1:A:260:VAL:HG21	1:A:284:LEU:HD21	1.98	0.44
1:A:142:ARG:CD	6:A:383:HOH:O	2.56	0.44
2:B:122:VAL:O	2:B:126:VAL:HG23	2.18	0.44
2:B:269:ASN:CG	2:B:272:SER:OG	2.56	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:189:ILE:HD11	1:A:205:HIS:CD2	2.52	0.44
2:B:34:ARG:HD3	2:B:284:PHE:CE1	2.52	0.44
2:B:309:PRO:HB2	2:B:399:PRO:HG2	2.00	0.44
2:B:337:GLU:HB3	2:B:341:MET:HE3	1.98	0.43
1:A:132:THR:HG23	2:B:147:TYR:CD2	2.52	0.43
1:A:312:ILE:O	1:A:316:VAL:HG23	2.19	0.43
2:B:178:LEU:HD23	2:B:422:GLY:HA2	2.00	0.43
1:A:198:LYS:HD3	2:B:294:LYS:HD3	1.99	0.43
2:B:119:PRO:O	2:B:122:VAL:N	2.52	0.43
2:B:127:CYS:SG	2:B:168:ALA:HA	2.58	0.43
2:B:277:VAL:O	2:B:280:ARG:HB2	2.19	0.43
2:B:212:SER:OG	2:B:213:LEU:N	2.51	0.43
2:B:398:HIS:CE1	6:B:576:HOH:O	2.71	0.43
2:B:118:ILE:HG22	2:B:122:VAL:HG22	2.00	0.43
1:A:363:LEU:O	1:A:364:GLN:C	2.56	0.43
1:A:337:ALA:O	1:A:340:LEU:N	2.52	0.43
6:A:509:HOH:O	2:B:329:MET:HG2	2.17	0.43
2:B:150:LEU:HD21	2:B:181:LEU:HD21	2.01	0.42
2:B:299:CYS:HB3	2:B:362:HIS:CD2	2.54	0.42
2:B:157:VAL:HG21	2:B:210:VAL:CG1	2.44	0.42
2:B:274:LEU:HA	2:B:311:LEU:HD13	2.00	0.42
1:A:163:PRO:HD2	6:A:473:HOH:O	2.19	0.42
2:B:348:GLY:O	2:B:358:ARG:HD3	2.19	0.42
6:A:511:HOH:O	2:B:38:ASP:OD1	2.22	0.42
1:A:364:GLN:O	1:A:365:SER:C	2.57	0.41
1:A:362:SER:HA	2:B:322:ALA:HB2	2.01	0.41
1:A:358:TYR:C	1:A:358:TYR:CD2	2.93	0.41
1:A:151:GLU:HA	1:A:151:GLU:OE1	2.20	0.41
2:B:386:VAL:CG2	2:B:393:VAL:HG13	2.47	0.41
1:A:155:ILE:HD13	1:A:171:HIS:HD2	1.84	0.41
1:A:138:ARG:NH2	6:A:394:HOH:O	2.22	0.41
1:A:214:ARG:HD3	6:A:466:HOH:O	2.20	0.41
1:A:250:TYR:O	1:A:252:ASP:O	2.39	0.41
1:A:312:ILE:HG22	1:A:344:LEU:HD11	2.03	0.41
1:A:153:ASN:ND2	6:A:446:HOH:O	2.53	0.41
2:B:160:LEU:HA	2:B:160:LEU:HD23	1.90	0.41
2:B:48:GLN:HE22	2:B:282:MET:HE2	1.86	0.41
1:A:75:ILE:HD11	1:A:105:ALA:HB1	2.01	0.41
2:B:205:TYR:CD2	4:B:428:FPP:H153	2.55	0.41
2:B:34:ARG:HD3	2:B:284:PHE:CZ	2.56	0.41
2:B:326:SER:C	2:B:327:HIS:ND1	2.74	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:142:ARG:NH1	1:A:148:LEU:HD11	2.35	0.40
1:A:112:ARG:HA	1:A:140:LEU:HD21	2.03	0.40
2:B:423:PHE:C	2:B:423:PHE:HD2	2.24	0.40
2:B:412:THR:O	2:B:413:THR:C	2.58	0.40

All (7) 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)
6:A:418:HOH:O	6:B:454:HOH:O[3_654]	1.63	0.57
6:B:500:HOH:O	6:B:515:HOH:O[3_655]	1.84	0.36
6:B:470:HOH:O	6:B:536:HOH:O[2_544]	2.08	0.12
6:A:428:HOH:O	6:B:519:HOH:O[3_655]	2.12	0.08
6:A:416:HOH:O	6:B:529:HOH:O[3_655]	2.13	0.07
2:B:88:GLN:OE1	6:A:486:HOH:O[4_545]	2.17	0.03
6:A:402:HOH:O	6:B:512:HOH:O[4_544]	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	313/379 (83%)	282 (90%)	25 (8%)	6 (2%)	10 4
2	B	401/426 (94%)	374 (93%)	23 (6%)	4 (1%)	19 13
All	All	714/805 (89%)	656 (92%)	48 (7%)	10 (1%)	14 7

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	252	ASP
1	A	256	LEU
1	A	329	ASN

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Mol	Chain	Res	Type
2	B	266	ARG
1	A	71	GLU
2	B	379	GLY
1	A	300	LEU
1	A	261	GLN
2	B	409	ILE
2	B	260	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	289/339 (85%)	267 (92%)	22 (8%)	16	12
2	B	340/362 (94%)	321 (94%)	19 (6%)	26	22
All	All	629/701 (90%)	588 (94%)	41 (6%)	21	17

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	55	PHE
1	A	59	ASP
1	A	67	ARG
1	A	109	ARG
1	A	121	ARG
1	A	145	GLN
1	A	156	ILE
1	A	218	ASN
1	A	220	LEU
1	A	252	ASP
1	A	287	ARG
1	A	301	ASP
1	A	302	LEU
1	A	307	SER
1	A	333	ILE
1	A	335	ASN

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Mol	Chain	Res	Type
1	A	336	LYS
1	A	342	GLU
1	A	352	ARG
1	A	354	GLU
1	A	358	TYR
1	A	362	SER
2	B	21	GLU
2	B	34	ARG
2	B	39	SER
2	B	70	ARG
2	B	87	ARG
2	B	137	ASP
2	B	263	LYS
2	B	266	ARG
2	B	267	SER
2	B	271	LYS
2	B	277	VAL
2	B	283	ARG
2	B	294	LYS
2	B	327	HIS
2	B	351	LEU
2	B	352	ASP
2	B	357	SER
2	B	393	VAL
2	B	423	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	153	ASN
1	A	170	HIS
1	A	201	HIS
1	A	211	GLN
1	A	218	ASN
1	A	221	GLN
1	A	239	GLN
1	A	246	ASN
1	A	285	GLN
1	A	294	ASN
1	A	325	ASN
2	B	48	GLN
2	B	134	GLN

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Mol	Chain	Res	Type
2	B	186	GLN
2	B	289	GLN
2	B	293	ASN
2	B	344	GLN
2	B	375	HIS
2	B	414	HIS

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

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	$\#\|Z\| > 2$
4	FPP	B	428	-	21,23,23	2.00	8 (38%)	27,31,31	1.71	8 (29%)
5	3PZ	B	429	3	38,42,42	3.47	8 (21%)	47,60,60	2.23	13 (27%)

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
4	FPP	B	428	-	-	0/25/25/25	0/0/0/0
5	3PZ	B	429	3	-	0/24/40/40	0/4/5/5

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	429	3PZ	C1-N2	-4.68	1.34	1.43
4	B	428	FPP	C6-C7	-3.56	1.40	1.50
4	B	428	FPP	C11-C12	-2.84	1.42	1.50
4	B	428	FPP	C1-C2	-2.66	1.40	1.49
5	B	429	3PZ	C11-N4	-2.40	1.33	1.38
5	B	429	3PZ	C25-S1	-2.15	1.73	1.76
4	B	428	FPP	PB-O3B	-2.09	1.47	1.54
5	B	429	3PZ	C14-N4	2.05	1.52	1.47
5	B	429	3PZ	O3-C28	2.28	1.49	1.42
4	B	428	FPP	O1-C1	2.44	1.46	1.43
4	B	428	FPP	C2-C3	2.81	1.38	1.33
4	B	428	FPP	C12-C13	3.02	1.41	1.32
4	B	428	FPP	C7-C8	3.72	1.40	1.33
5	B	429	3PZ	O2-S1	6.36	1.51	1.43
5	B	429	3PZ	O1-S1	7.57	1.53	1.43
5	B	429	3PZ	S1-N1	17.37	1.88	1.63

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	429	3PZ	O2-S1-O1	-6.87	107.62	119.47
5	B	429	3PZ	C7-C2-C3	-6.63	110.44	119.28
5	B	429	3PZ	N3-C13-N4	-4.28	106.49	112.28
5	B	429	3PZ	C28-O3-C22	-3.73	108.78	117.51
4	B	428	FPP	O3A-PA-O1	-3.17	94.52	102.94
5	B	429	3PZ	C15-C8-N1	-2.65	108.91	112.87
4	B	428	FPP	O2B-PB-O1B	-2.62	102.14	110.58
4	B	428	FPP	PA-O3A-PB	-2.22	125.22	132.67
5	B	429	3PZ	C3-C4-C29	-2.13	116.82	119.51
4	B	428	FPP	O2A-PA-O3A	2.05	114.40	105.09
4	B	428	FPP	O3B-PB-O2B	2.06	115.23	107.38
5	B	429	3PZ	C12-N3-C13	2.14	109.09	105.71
5	B	429	3PZ	O1-S1-N1	2.18	111.60	106.97
4	B	428	FPP	C4-C3-C5	2.52	119.25	115.41
4	B	428	FPP	O3B-PB-O1B	2.62	119.00	110.58
5	B	429	3PZ	C3-C2-C1	2.80	121.20	118.93
5	B	429	3PZ	C19-C15-C8	3.12	118.91	113.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	429	3PZ	C7-C2-C1	3.80	128.33	122.44
5	B	429	3PZ	C7-N1-S1	4.04	126.14	118.31
4	B	428	FPP	C10-C8-C9	4.11	121.68	115.41
5	B	429	3PZ	C25-S1-N1	4.60	114.90	107.38

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	428	FPP	2	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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^{th} 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	315/379 (83%)	0.52	20 (6%)	23	31	20, 45, 89, 123	0
2	B	403/426 (94%)	0.33	13 (3%)	51	60	19, 37, 73, 97	0
All	All	718/805 (89%)	0.41	33 (4%)	36	45	19, 40, 84, 123	0

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	422	GLY	5.9
2	B	423	PHE	5.0
2	B	64	PHE	4.7
1	A	55	PHE	4.4
1	A	305	SER	4.3
2	B	380	ALA	4.2
2	B	412	THR	3.7
1	A	333	ILE	3.4
1	A	335	ASN	3.4
1	A	369	ARG	3.4
1	A	220	LEU	3.3
1	A	302	LEU	3.3
1	A	217	ASP	3.3
1	A	320	GLU	3.0
1	A	256	LEU	2.7
1	A	341	CYS	2.6
1	A	251	SER	2.6
1	A	366	LYS	2.5
2	B	415	PHE	2.5
2	B	377	GLY	2.5
1	A	287	ARG	2.5
2	B	409	ILE	2.4
1	A	368	SER	2.4
1	A	360	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
2	B	120	GLN	2.3
1	A	250	TYR	2.3
2	B	168	ALA	2.2
1	A	255	VAL	2.2
2	B	420	VAL	2.2
2	B	321	PRO	2.2
2	B	416	LEU	2.0
1	A	306	HIS	2.0
1	A	304	PRO	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, 95^{th} 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^2)	Q<0.9
4	FPP	B	428	24/24	0.96	0.15	3.31	27,35,46,53	0
5	3PZ	B	429	38/38	0.91	0.13	1.17	20,31,67,71	0
3	ZN	B	1	1/1	1.00	0.12	0.02	24,24,24,24	0

6.5 Other polymers (i)

There are no such residues in this entry.