Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 05:47 AM GMT

PDB ID	:	2TSY
Title	:	CRYSTAL STRUCTURES OF MUTANT (BETAK87T) TRYPTOPHAN SYNTHASE ALPHA2 BETA2 COMPLEX WITH LIGANDS BOUND TO THE ACTIVE SITES OF THE ALPHA AND BETA SUBUNITS REVEAL LIGAND-INDUCED CONFORMATIONAL CHANGES
Authors	:	Rhee, S.; Parris, K.D.; Hyde, C.C.; Ahmed, S.A.; Miles, E.W.; Davies, D.R.
Deposited on	:	1997-01-03
Resolution	:	2.50 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:

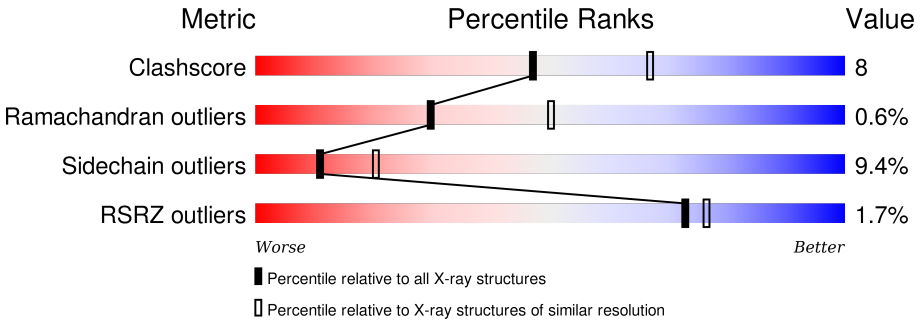
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.50 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))
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

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	268	4% 71% 23%
2	B	397	71% 24%

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	G3P	A	271	X	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 5082 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 TRYPTOPHAN SYNTHASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	262	Total	C	N	O	S	0	0	0
			1976	1253	343	372	8			

- Molecule 2 is a protein called TRYPTOPHAN SYNTHASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	389	Total	C	N	O	S	0	0	0
			2948	1853	517	559	19			

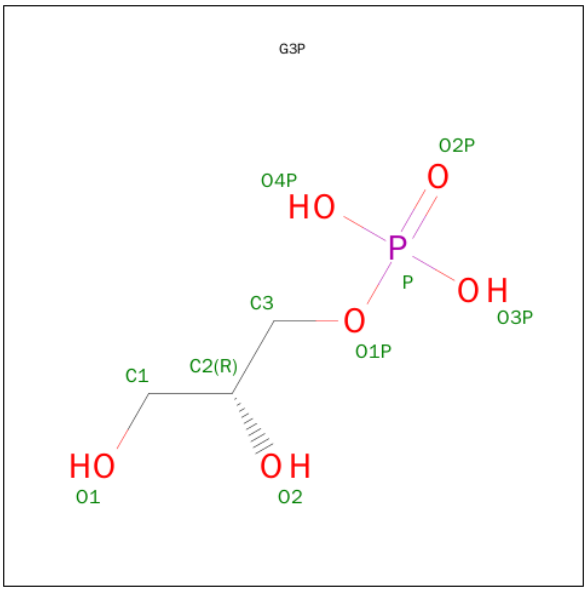
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	87	THR	LYS	ENGINEERED	UNP P0A2K1
B	396	LEU	GLU	CONFLICT	UNP P0A2K1

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

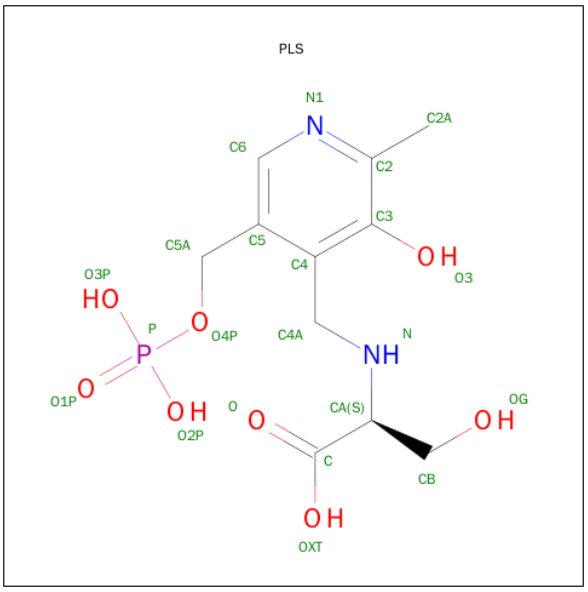
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Na	0	0
			1	1		

- Molecule 4 is SN-GLYCEROL-3-PHOSPHATE (three-letter code: G3P) (formula: $C_3H_9O_6P$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	P		
4	A	1	10	3	6	1	0	0

- Molecule 5 is [3-HYDROXY-2-METHYL-5-PHOSPHONOOXYMETHYL-PYRIDIN-4-YL METHYL]-SERINE (three-letter code: PLS) (formula: $C_{11}H_{17}N_2O_8P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
5	B	1	22	11	2	8	1	0	0

- Molecule 6 is water.

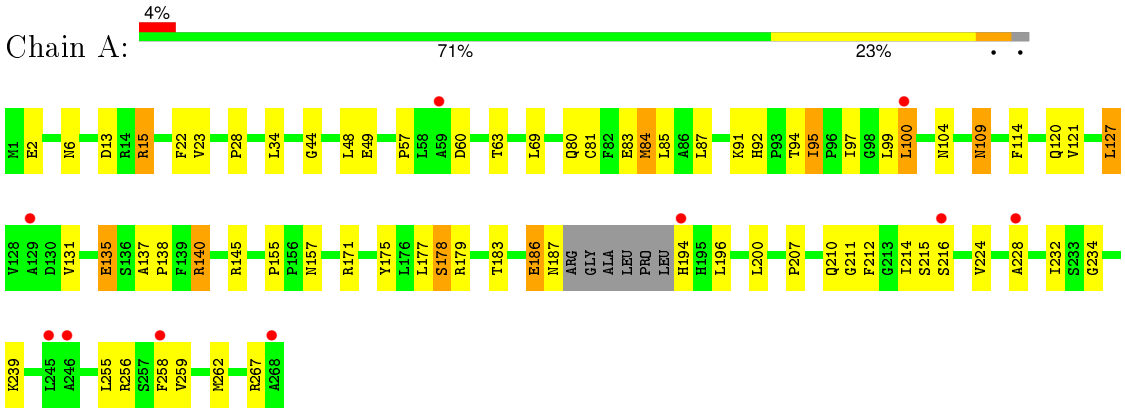
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	38	Total O 38 38	0	0
6	B	87	Total O 87 87	0	0

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.

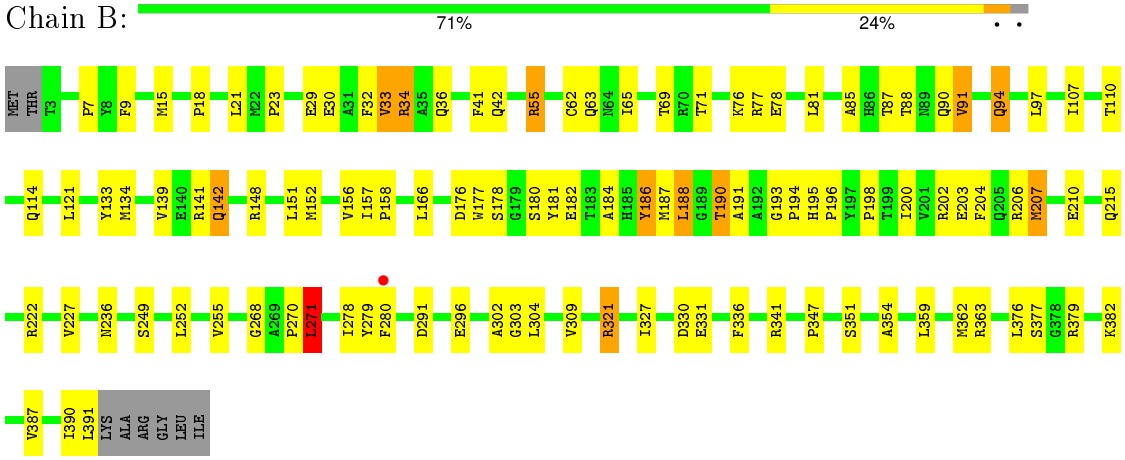
- Molecule 1: TRYPTOPHAN SYNTHASE

Chain A:



- Molecule 2: TRYPTOPHAN SYNTHASE

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	185.70Å 62.60Å 67.90Å 90.00° 94.40° 90.00°	Depositor
Resolution (Å)	8.00 – 2.50 31.87 – 2.51	Depositor EDS
% Data completeness (in resolution range)	89.5 (8.00-2.50) 90.8 (31.87-2.51)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$< I/\sigma(I) >$ [1]	4.61 (at 2.51Å)	Xtriage
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.187 , (Not available) 0.172 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å^2)	41.0	Xtriage
Anisotropy	0.710	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 116.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 24346 reflections	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	5082	wwPDB-VP
Average B, all atoms (Å^2)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.07% 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: G3P, PLS, NA

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	0.74	0/2014	1.43	17/2733 (0.6%)
2	B	0.88	0/3006	1.60	35/4063 (0.9%)
All	All	0.83	0/5020	1.54	52/6796 (0.8%)

There are no bond length outliers.

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	77	ARG	NE-CZ-NH2	-9.52	115.54	120.30
2	B	15	MET	CG-SD-CE	-9.49	85.02	100.20
2	B	202	ARG	NE-CZ-NH2	-9.32	115.64	120.30
2	B	177	TRP	CD1-CG-CD2	8.91	113.43	106.30
2	B	152	MET	CG-SD-CE	-8.85	86.04	100.20
2	B	207	MET	CG-SD-CE	-8.63	86.39	100.20
1	A	84	MET	CA-CB-CG	8.04	126.97	113.30
1	A	23	VAL	CG1-CB-CG2	-7.91	98.24	110.90
2	B	148	ARG	NE-CZ-NH1	7.88	124.24	120.30
1	A	179	ARG	NE-CZ-NH2	-7.70	116.45	120.30
2	B	55	ARG	CA-CB-CG	7.58	130.08	113.40
1	A	186	GLU	CA-C-N	-7.51	100.68	117.20
1	A	121	VAL	CG1-CB-CG2	-7.39	99.07	110.90
2	B	77	ARG	NE-CZ-NH1	7.37	123.98	120.30
2	B	222	ARG	NE-CZ-NH1	-7.35	116.63	120.30
1	A	145	ARG	NE-CZ-NH2	-7.17	116.72	120.30
1	A	179	ARG	NE-CZ-NH1	7.08	123.84	120.30
1	A	145	ARG	NE-CZ-NH1	7.04	123.82	120.30
2	B	177	TRP	CE2-CD2-CG	-6.92	101.77	107.30
2	B	271	LEU	CA-CB-CG	6.91	131.20	115.30
2	B	91	VAL	CG1-CB-CG2	-6.88	99.88	110.90
2	B	55	ARG	NE-CZ-NH1	6.69	123.64	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	186	GLU	O-C-N	6.68	133.38	122.70
1	A	140	ARG	NE-CZ-NH1	-6.66	116.97	120.30
2	B	321	ARG	NE-CZ-NH1	6.45	123.52	120.30
2	B	34	ARG	NE-CZ-NH2	6.16	123.38	120.30
2	B	176	ASP	CB-CG-OD1	6.16	123.84	118.30
2	B	341	ARG	CA-C-N	6.06	130.52	117.20
2	B	88	THR	CA-C-N	5.99	130.37	117.20
2	B	222	ARG	NE-CZ-NH2	5.87	123.24	120.30
2	B	177	TRP	CG-CD1-NE1	-5.74	104.36	110.10
2	B	133	TYR	CB-CG-CD2	-5.63	117.62	121.00
1	A	81	CYS	CA-CB-SG	-5.59	103.94	114.00
2	B	186	TYR	CB-CG-CD2	-5.45	117.73	121.00
2	B	33	VAL	CG1-CB-CG2	-5.45	102.19	110.90
1	A	177	LEU	CA-C-N	-5.44	105.23	117.20
2	B	390	ILE	CA-C-N	-5.42	105.28	117.20
2	B	302	ALA	CA-C-N	5.34	126.87	116.20
2	B	379	ARG	NE-CZ-NH1	5.33	122.97	120.30
1	A	256	ARG	NE-CZ-NH2	5.33	122.96	120.30
1	A	171	ARG	NE-CZ-NH1	-5.31	117.64	120.30
1	A	211	GLY	N-CA-C	5.29	126.33	113.10
2	B	141	ARG	NE-CZ-NH2	5.27	122.93	120.30
2	B	9	PHE	N-CA-C	-5.25	96.83	111.00
2	B	330	ASP	CB-CG-OD1	5.20	122.98	118.30
2	B	391	LEU	CA-CB-CG	5.20	127.25	115.30
1	A	171	ARG	NE-CZ-NH2	5.16	122.88	120.30
2	B	151	LEU	CA-CB-CG	5.15	127.15	115.30
1	A	194	HIS	CA-C-N	5.12	128.46	117.20
2	B	121	LEU	CA-CB-CG	5.06	126.93	115.30
2	B	279	TYR	CB-CG-CD1	-5.04	117.98	121.00
2	B	148	ARG	NE-CZ-NH2	-5.02	117.79	120.30

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	1976	0	1977	28	0
2	B	2948	0	2920	48	0
3	B	1	0	0	0	0
4	A	10	0	4	4	0
5	B	22	0	13	2	0
6	A	38	0	0	0	0
6	B	87	0	0	1	0
All	All	5082	0	4914	74	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 8.

All (74) 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)
4:A:271:G3P:C3	4:A:271:G3P:O1P	1.68	1.37
1:A:210:GLN:HE21	1:A:214:ILE:HD11	1.47	0.79
2:B:21:LEU:HD21	2:B:178:SER:HA	1.69	0.75
1:A:22:PHE:HB3	1:A:234:GLY:HA2	1.67	0.74
1:A:92:HIS:HB3	1:A:95:ILE:HD11	1.72	0.70
2:B:359:LEU:O	2:B:363:ARG:HG2	1.92	0.68
2:B:69:THR:HG22	2:B:71:THR:H	1.59	0.67
2:B:271:LEU:HB2	2:B:309:VAL:HG11	1.79	0.63
1:A:175:TYR:CE2	1:A:232:ILE:HD12	2.35	0.62
4:A:271:G3P:C3	4:A:271:G3P:P	2.87	0.61
2:B:91:VAL:HG13	2:B:187:MET:SD	2.41	0.61
1:A:100:LEU:HD23	1:A:127:LEU:HB3	1.84	0.60
2:B:134:MET:HG2	2:B:139:VAL:HG23	1.83	0.60
1:A:157:ASN:HD22	2:B:23:PRO:HG2	1.67	0.59
2:B:69:THR:HG21	2:B:362:MET:CG	2.34	0.57
2:B:271:LEU:O	2:B:271:LEU:HD12	2.04	0.57
1:A:157:ASN:ND2	2:B:23:PRO:HG2	2.20	0.57
1:A:183:THR:HG22	4:A:271:G3P:H32	1.88	0.56
1:A:183:THR:CG2	4:A:271:G3P:H32	2.35	0.56
2:B:78:GLU:HB2	2:B:377:SER:HA	1.87	0.56
2:B:107:ILE:HD11	2:B:184:ALA:HB1	1.88	0.56
2:B:327:ILE:HG23	2:B:331:GLU:HB2	1.88	0.55
2:B:303:GLY:O	5:B:398:PLS:H5A1	2.05	0.55
1:A:57:PRO:HB2	1:A:60:ASP:HB2	1.89	0.55
2:B:69:THR:HG21	2:B:362:MET:HG3	1.89	0.54
2:B:30:GLU:O	2:B:34:ARG:HG3	2.07	0.54
2:B:29:GLU:HB2	2:B:196:PRO:HG3	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:186:TYR:CE2	2:B:188:LEU:HG	2.43	0.53
1:A:258:PHE:O	1:A:262:MET:HG2	2.09	0.52
1:A:104:ASN:HD22	2:B:278:ILE:H	1.57	0.51
1:A:85:LEU:HD11	1:A:99:LEU:HD21	1.93	0.51
2:B:62:CYS:SG	2:B:65:ILE:HD11	2.51	0.50
2:B:255:VAL:HG21	2:B:354:ALA:HA	1.94	0.50
2:B:193:GLY:HA2	2:B:280:PHE:O	2.12	0.50
2:B:76:LYS:HZ2	2:B:215:GLN:HE22	1.59	0.49
2:B:142:GLN:OE1	2:B:382:LYS:HD2	2.12	0.49
2:B:94:GLN:HB3	2:B:187:MET:HE2	1.94	0.48
1:A:224:VAL:HA	1:A:228:ALA:O	2.12	0.48
2:B:90:GLN:HE21	2:B:94:GLN:NE2	2.12	0.48
2:B:94:GLN:HB3	2:B:187:MET:CE	2.43	0.48
2:B:194:PRO:HG3	6:B:427:HOH:O	2.11	0.48
2:B:303:GLY:HA3	5:B:398:PLS:H4A2	1.95	0.47
1:A:34:LEU:HD21	1:A:84:MET:HB2	1.95	0.47
2:B:69:THR:HG21	2:B:362:MET:HG2	1.96	0.47
1:A:104:ASN:ND2	2:B:278:ILE:H	2.13	0.47
2:B:87:THR:HG21	2:B:114:GLN:O	2.14	0.47
2:B:157:ILE:HA	2:B:158:PRO:HD3	1.74	0.46
2:B:190:THR:OG1	2:B:191:ALA:N	2.47	0.46
1:A:255:LEU:O	1:A:259:VAL:HG23	2.16	0.46
2:B:41:PHE:HD2	2:B:42:GLN:NE2	2.14	0.45
1:A:137:ALA:HB3	1:A:138:PRO:HD3	1.97	0.45
2:B:81:LEU:HD23	2:B:85:ALA:O	2.16	0.45
1:A:22:PHE:HD2	1:A:49:GLU:HB3	1.81	0.45
2:B:29:GLU:O	2:B:33:VAL:HG23	2.17	0.45
1:A:91:LYS:HG3	1:A:92:HIS:CD2	2.52	0.44
2:B:376:LEU:HD12	2:B:376:LEU:HA	1.85	0.44
1:A:131:VAL:HG13	1:A:135:GLU:HB3	2.00	0.44
2:B:206:ARG:O	2:B:210:GLU:HG3	2.17	0.44
1:A:109:ASN:HD21	1:A:114:PHE:HB2	1.82	0.44
2:B:180:SER:O	2:B:182:GLU:N	2.51	0.43
2:B:110:THR:HG22	2:B:134:MET:HB2	2.01	0.43
2:B:336:PHE:CE2	2:B:387:VAL:HG11	2.53	0.43
1:A:15:ARG:NE	1:A:15:ARG:HA	2.34	0.43
2:B:268:GLY:C	2:B:270:PRO:HD2	2.38	0.43
2:B:32:PHE:CD1	2:B:200:ILE:HG12	2.55	0.42
1:A:48:LEU:HB2	1:A:97:ILE:HG22	2.02	0.41
2:B:41:PHE:HD2	2:B:42:GLN:HE21	1.68	0.41
1:A:95:ILE:HD13	1:A:95:ILE:H	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:227:VAL:HG22	2:B:252:LEU:HD23	2.02	0.41
2:B:7:PRO:HB3	2:B:195:HIS:CG	2.56	0.41
2:B:90:GLN:HA	2:B:204:PHE:HB3	2.02	0.41
1:A:137:ALA:HA	1:A:140:ARG:HG2	2.03	0.41
1:A:178:SER:OG	1:A:212:PHE:N	2.54	0.40
1:A:200:LEU:HD12	1:A:200:LEU:HA	1.99	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	258/268 (96%)	230 (89%)	25 (10%)	3 (1%)	16 29
2	B	387/397 (98%)	364 (94%)	22 (6%)	1 (0%)	46 68
All	All	645/665 (97%)	594 (92%)	47 (7%)	4 (1%)	30 50

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	181	TYR
1	A	15	ARG
1	A	13	ASP
1	A	44	GLY

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	204/208 (98%)	179 (88%)	25 (12%)	6 11
2	B	305/311 (98%)	282 (92%)	23 (8%)	17 31
All	All	509/519 (98%)	461 (91%)	48 (9%)	11 20

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	GLU
1	A	6	ASN
1	A	28	PRO
1	A	63	THR
1	A	69	LEU
1	A	80	GLN
1	A	83	GLU
1	A	87	LEU
1	A	94	THR
1	A	95	ILE
1	A	100	LEU
1	A	109	ASN
1	A	120	GLN
1	A	127	LEU
1	A	135	GLU
1	A	155	PRO
1	A	178	SER
1	A	186	GLU
1	A	187	ASN
1	A	196	LEU
1	A	207	PRO
1	A	215	SER
1	A	216	SER
1	A	239	LYS
1	A	267	ARG
2	B	18	PRO
2	B	36	GLN
2	B	55	ARG
2	B	63	GLN
2	B	94	GLN
2	B	97	LEU
2	B	142	GLN
2	B	156	VAL
2	B	166	LEU

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Mol	Chain	Res	Type
2	B	188	LEU
2	B	190	THR
2	B	198	PRO
2	B	203	GLU
2	B	207	MET
2	B	236	ASN
2	B	249	SER
2	B	271	LEU
2	B	291	ASP
2	B	296	GLU
2	B	304	LEU
2	B	321	ARG
2	B	347	PRO
2	B	351	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	104	ASN
1	A	109	ASN
1	A	210	GLN
2	B	36	GLN
2	B	42	GLN
2	B	94	GLN
2	B	195	HIS
2	B	215	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)

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	G3P	A	271	-	9,9,9	4.18	6 (66%)	10,12,12	2.29	4 (40%)
5	PLS	B	398	-	19,22,22	2.55	8 (42%)	23,31,31	3.90	11 (47%)

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	G3P	A	271	-	1/1/2/2	0/8/8/8	0/0/0/0
5	PLS	B	398	-	-	0/13/17/17	0/1/1/1

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	271	G3P	C1-C2	-8.25	1.20	1.52
5	B	398	PLS	P-O1P	-5.60	1.32	1.51
5	B	398	PLS	P-O4P	-5.30	1.42	1.60
4	A	271	G3P	P-O3P	-4.63	1.38	1.54
5	B	398	PLS	C4A-N	-2.98	1.37	1.46
5	B	398	PLS	C5-C4	-2.55	1.36	1.40
5	B	398	PLS	P-O3P	-2.34	1.46	1.54
5	B	398	PLS	C6-C5	2.11	1.42	1.37
5	B	398	PLS	C3-C4	2.14	1.43	1.40
4	A	271	G3P	O1-C1	2.79	1.54	1.42
4	A	271	G3P	O2-C2	3.06	1.52	1.43
4	A	271	G3P	P-O2P	3.10	1.61	1.51
5	B	398	PLS	C3-C2	4.89	1.44	1.40
4	A	271	G3P	O1P-C3	5.73	1.68	1.44

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	271	G3P	O3P-P-O2P	-3.34	99.81	110.58
4	A	271	G3P	O2-C2-C1	-3.05	94.66	108.65
5	B	398	PLS	C5-C6-N1	-2.52	119.49	123.86
5	B	398	PLS	C4A-C4-C5	-2.35	117.61	119.71
5	B	398	PLS	O2P-P-O1P	-2.24	103.37	110.58
5	B	398	PLS	O2P-P-O4P	-2.21	100.20	106.56
5	B	398	PLS	O3P-P-O1P	-2.00	104.14	110.58
5	B	398	PLS	C6-N1-C2	2.35	124.07	119.28
4	A	271	G3P	O1-C1-C2	3.08	125.13	110.18
5	B	398	PLS	OG-CB-CA	3.70	118.91	111.61
4	A	271	G3P	C3-C2-C1	3.75	126.24	111.08
5	B	398	PLS	O3-C3-C2	4.22	125.00	117.66
5	B	398	PLS	O4P-C5A-C5	4.40	116.26	108.99
5	B	398	PLS	O3P-P-O4P	9.90	135.08	106.56
5	B	398	PLS	C4A-N-CA	12.56	133.01	113.81

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	A	271	G3P	C2

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	271	G3P	4	0
5	B	398	PLS	2	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, 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	262/268 (97%)	-0.07	10 (3%) 44 49	21, 49, 86, 106	1 (0%)
2	B	389/397 (97%)	-0.51	1 (0%) 94 95	12, 28, 51, 84	2 (0%)
All	All	651/665 (97%)	-0.33	11 (1%) 73 76	12, 36, 74, 106	3 (0%)

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	268	ALA	3.7
1	A	246	ALA	3.5
1	A	100	LEU	3.4
1	A	245	LEU	3.0
1	A	194	HIS	2.8
1	A	216	SER	2.5
1	A	258	PHE	2.5
1	A	129	ALA	2.0
1	A	228	ALA	2.0
2	B	280	PHE	2.0
1	A	59	ALA	2.0

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands (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
5	PLS	B	398	22/22	0.98	0.24	1.60	29,35,52,53	0
4	G3P	A	271	10/10	0.93	0.24	0.87	54,59,65,68	0
3	NA	B	400	1/1	0.97	0.06	-1.64	26,26,26,26	0

6.5 Other polymers (i)

There are no such residues in this entry.