Full wwPDB X-ray Structure Validation Report ⓘ

Aug 22, 2020 – 08:14 PM BST

PDB ID	:	3R9A
Title	:	Human alanine-glyoxylate aminotransferase in complex with the TPR domain of human PEX5P
Authors	:	Fodor, K.; Wilmanns, M.
Deposited on	:	2011-03-25
Resolution	:	2.35 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
https://www.wwpdb.org/validation/2017/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:

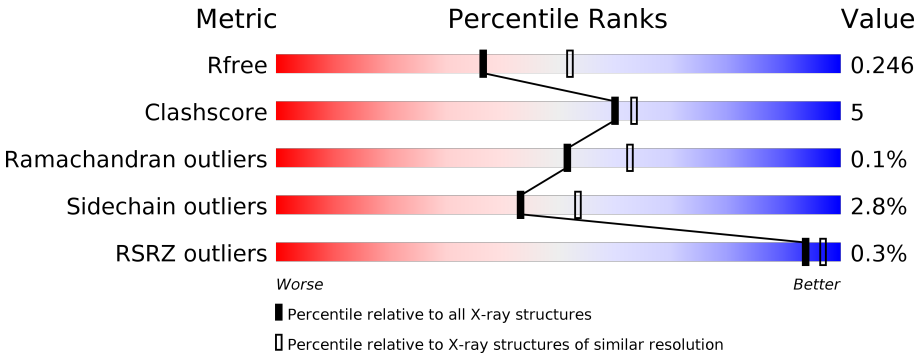
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

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 2.35 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}	130704	1164 (2.36-2.36)
Clashscore	141614	1232 (2.36-2.36)
Ramachandran outliers	138981	1211 (2.36-2.36)
Sidechain outliers	138945	1212 (2.36-2.36)
RSRZ outliers	127900	1150 (2.36-2.36)

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 respectively. 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	394	87% 10% • •
1	C	394	88% 10% • •
2	B	328	% 79% 8% • 12%
2	D	328	79% 9% • 11%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 11436 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 Serine–pyruvate aminotransferase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	387	Total	C	N	O	P	S	0	1	0
			2999	1917	520	545	1	16			
1	C	389	Total	C	N	O	P	S	0	3	0
			3014	1925	525	546	1	17			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	EXPRESSION TAG	UNP P21549
A	0	ALA	-	EXPRESSION TAG	UNP P21549
C	-1	GLY	-	EXPRESSION TAG	UNP P21549
C	0	ALA	-	EXPRESSION TAG	UNP P21549

- Molecule 2 is a protein called Peroxisomal targeting signal 1 receptor.

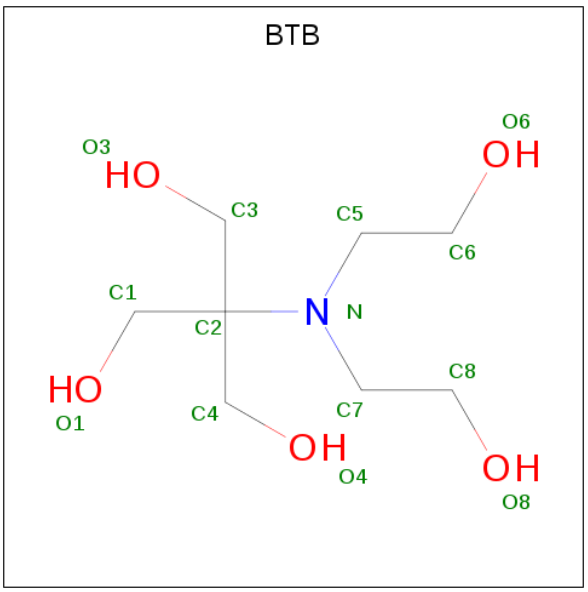
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	289	Total	C	N	O	S	0	1	0
			2274	1427	399	437	11			
2	D	292	Total	C	N	O	S	0	2	0
			2304	1452	400	441	11			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	312	GLY	-	EXPRESSION TAG	UNP P50542
B	313	ALA	-	EXPRESSION TAG	UNP P50542
B	314	MET	-	EXPRESSION TAG	UNP P50542
D	312	GLY	-	EXPRESSION TAG	UNP P50542
D	313	ALA	-	EXPRESSION TAG	UNP P50542
D	314	MET	-	EXPRESSION TAG	UNP P50542

- Molecule 3 is 2-[BIS-(2-HYDROXY-ETHYL)-AMINO]-2-HYDROXYMETHYL-PROPAN

E-1,3-DIOL (three-letter code: BTB) (formula: $C_8H_{19}NO_5$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	C	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 4 is water.

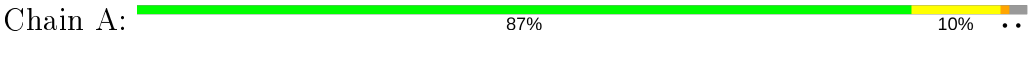
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	307	Total	O	0	0
			307	307		
4	B	186	Total	O	0	0
			186	186		
4	C	204	Total	O	0	0
			204	204		
4	D	134	Total	O	0	0
			134	134		

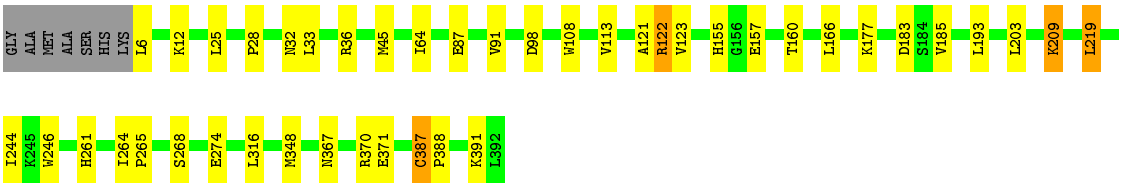
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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: Serine–pyruvate aminotransferase

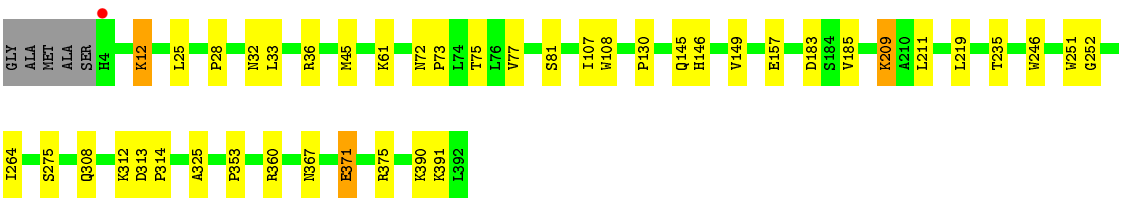
Chain A:





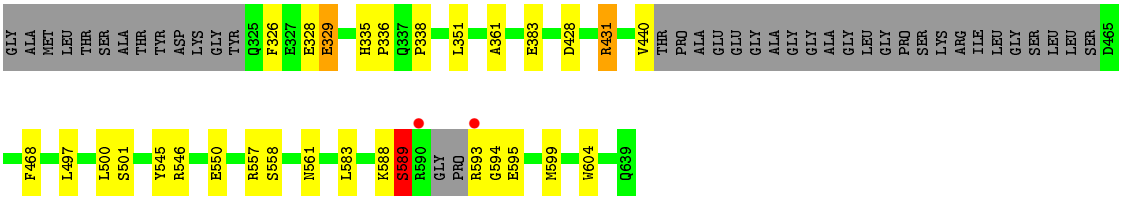
- Molecule 1: Serine–pyruvate aminotransferase

Chain C:



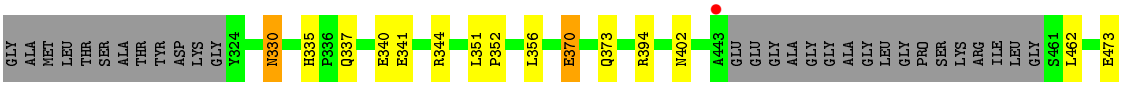
- Molecule 2: Peroxisomal targeting signal 1 receptor

Chain B:



- Molecule 2: Peroxisomal targeting signal 1 receptor

Chain D:




N534
G535
N536
E539
Y545
R546
R547
Q552
P553
G554
R557
Y560
N561
L562
G563
I564
S589
ARG
GLY
PRO
ARG
GLY
GLU
GLY
G597
N602
I603
W604
S612
Y620
R626
Q639

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	59.37Å 99.16Å 127.70Å 90.00° 96.66° 90.00°	Depositor
Resolution (Å)	78.09 – 2.35 78.12 – 2.35	Depositor EDS
% Data completeness (in resolution range)	99.7 (78.09-2.35) 99.6 (78.12-2.35)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.77 (at 2.34Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.184 , 0.239 0.191 , 0.246	Depositor DCC
R_{free} test set	3096 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å^2)	29.3	Xtriage
Anisotropy	0.058	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 33.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	11436	wwPDB-VP
Average B, all atoms (Å^2)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.46% 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, 0.333 respectively for untwinned datasets, and 0.375, 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: LLP, BTB

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.42	0/3045	0.57	0/4130
1	C	0.38	0/3065	0.54	0/4161
2	B	0.44	0/2319	0.54	0/3141
2	D	0.41	0/2354	0.53	0/3193
All	All	0.41	0/10783	0.55	0/14625

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	329	GLU	Peptide

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	2999	0	3036	28	0
1	C	3014	0	3026	30	0
2	B	2274	0	2217	23	0
2	D	2304	0	2261	22	0
3	C	14	0	19	2	0
4	A	307	0	0	4	0
4	B	186	0	0	0	0
4	C	204	0	0	1	0
4	D	134	0	0	4	0
All	All	11436	0	10559	97	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 (97) 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:25:LEU:H	1:A:32:ASN:HD21	1.24	0.86
2:B:583:LEU:HB3	2:B:599:MET:HE3	1.57	0.85
2:B:588:LYS:HA	2:B:589:SER:HB2	1.58	0.84
2:D:552:GLN:HE21	2:D:554:GLY:H	1.25	0.81
1:C:183:ASP:OD1	1:C:209:LLP:H2'2	1.86	0.76
1:C:130:PRO:HG3	1:C:353:PRO:HB2	1.66	0.76
2:D:335:HIS:CE1	2:D:341:GLU:HG3	2.22	0.74
1:C:25:LEU:H	1:C:32:ASN:HD21	1.37	0.73
1:A:32:ASN:HD22	1:A:367:ASN:HD21	1.34	0.72
4:A:562:HOH:O	1:C:81:SER:HB3	1.92	0.70
2:D:560:TYR:CE2	2:D:564[A]:ILE:HD11	2.26	0.69
1:A:108:TRP:CD1	1:A:209:LLP:H2'3	2.27	0.69
2:B:588:LYS:HA	2:B:589:SER:CB	2.24	0.68
1:A:87:GLU:O	1:A:91:VAL:HG23	1.93	0.67
2:B:328:GLU:HG3	2:B:329:GLU:N	2.10	0.67
1:A:183:ASP:OD1	1:A:209:LLP:H2'2	2.00	0.62
2:D:597:GLY:HA3	4:D:892:HOH:O	1.99	0.61
1:C:32:ASN:HD22	1:C:367:ASN:HD21	1.51	0.59
1:A:121:ALA:HA	1:A:122:ARG:HB2	1.87	0.57
1:A:391:LYS:HB2	2:B:557:ARG:HD2	1.85	0.57
2:D:373:GLN:HE21	2:D:402:ASN:HD21	1.51	0.57
1:C:308:GLN:HG3	1:C:325:ALA:HB3	1.85	0.56
1:A:33:LEU:HD21	1:C:45:MET:CE	2.35	0.56
1:A:371:GLU:HB2	4:A:601:HOH:O	2.06	0.55
1:C:25:LEU:H	1:C:32:ASN:ND2	2.03	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:157:GLU:HG3	1:A:160:THR:OG1	2.06	0.55
2:B:594:GLY:HA2	2:B:595:GLU:HB2	1.89	0.54
2:B:588:LYS:CA	2:B:589:SER:HB2	2.36	0.53
1:C:77:VAL:HB	1:C:251:TRP:CZ2	2.44	0.53
2:B:383:GLU:OE1	2:B:557:ARG:HD3	2.08	0.53
2:D:335:HIS:HD2	2:D:337:GLN:H	1.56	0.52
2:D:561:ASN:HA	2:D:564[A]:ILE:HD12	1.90	0.52
1:A:387:CYS:N	1:A:388:PRO:CD	2.73	0.52
2:D:335:HIS:NE2	2:D:341:GLU:HG3	2.24	0.52
2:D:602:ASN:HB2	4:D:673:HOH:O	2.09	0.52
1:C:12:LYS:H	1:C:12:LYS:HE3	1.74	0.52
2:B:545:TYR:CZ	2:B:561:ASN:HB3	2.45	0.51
1:A:387:CYS:N	1:A:388:PRO:HD2	2.26	0.51
2:B:468:PHE:CZ	2:B:501:SER:HB3	2.46	0.51
1:A:193:LEU:HD21	1:A:203:LEU:HD21	1.94	0.50
1:A:246:TRP:HB3	1:A:261:HIS:CD2	2.47	0.50
2:B:599:MET:CE	2:B:604:TRP:CZ2	2.96	0.49
2:D:604:TRP:CD2	2:D:626:ARG:HD2	2.47	0.49
1:A:25:LEU:H	1:A:32:ASN:ND2	2.00	0.48
1:C:12:LYS:HE3	1:C:12:LYS:N	2.27	0.48
1:A:265:PRO:HB2	1:A:268:SER:HB2	1.96	0.48
1:A:6:LEU:N	4:A:649:HOH:O	2.47	0.48
1:A:64:ILE:HG12	1:A:219:LEU:HD13	1.96	0.47
2:B:599:MET:HE2	2:B:604:TRP:CZ2	2.49	0.47
1:C:185:VAL:HB	1:C:209:LLP:C2	2.44	0.47
1:C:390:LYS:HD3	2:D:534:ASN:OD1	2.14	0.47
2:D:547:ARG:HD2	4:D:655:HOH:O	2.15	0.46
1:C:246:TRP:HA	3:C:393:BTB:H71	1.98	0.46
1:A:45:MET:CE	1:C:33:LEU:HD21	2.46	0.46
1:C:391:LYS:CB	2:D:557:ARG:HD2	2.46	0.46
2:B:593:ARG:HA	2:B:594:GLY:HA2	1.80	0.45
2:D:612:SER:HA	2:D:620:TYR:OH	2.17	0.45
2:B:338:PRO:HB2	2:B:361:ALA:HB2	1.99	0.45
1:A:391:LYS:CB	2:B:557:ARG:HD2	2.46	0.45
2:D:370:GLU:HB2	4:D:786:HOH:O	2.17	0.45
2:D:341:GLU:OE2	2:D:344:ARG:NE	2.45	0.44
2:B:431:ARG:HB3	2:B:440:VAL:HG21	1.99	0.44
1:C:107:ILE:HG23	1:C:108:TRP:CD2	2.52	0.44
1:A:244:ILE:HA	1:A:244:ILE:HD12	1.87	0.44
1:C:12:LYS:H	1:C:12:LYS:CE	2.30	0.44
2:B:335:HIS:HA	2:B:336:PRO:HD3	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:391:LYS:HB2	2:D:557:ARG:HD2	1.99	0.44
1:C:28:PRO:HG3	1:C:360:ARG:NH2	2.33	0.44
1:C:108:TRP:CD1	1:C:209:LLP:H2'3	2.54	0.43
2:D:341:GLU:HG2	2:D:344:ARG:NH2	2.33	0.43
2:D:351:LEU:HB2	2:D:352:PRO:HD3	1.99	0.43
1:C:211:LEU:O	1:C:275:SER:HB2	2.19	0.43
2:D:337:GLN:HB3	2:D:340:GLU:HB2	2.01	0.42
1:A:28:PRO:CD	1:A:348:MET:HG3	2.49	0.42
1:C:252:GLY:HA2	4:C:468:HOH:O	2.19	0.42
1:A:370:ARG:HD3	4:A:396:HOH:O	2.20	0.42
1:A:98:ASP:O	1:A:122:ARG:HB2	2.19	0.42
1:C:145:GLN:HE21	1:C:146:HIS:CE1	2.37	0.42
1:A:122:ARG:HA	1:A:122:ARG:HD3	1.79	0.42
1:C:72:ASN:HA	1:C:73:PRO:HD3	1.93	0.42
1:C:209:LLP:O3	1:C:209:LLP:NZ	2.52	0.42
2:D:330:ASN:ND2	2:D:356:LEU:HB3	2.34	0.42
2:B:546:ARG:O	2:B:550:GLU:HG3	2.20	0.41
1:A:185:VAL:HB	1:A:209:LLP:C2	2.49	0.41
2:B:599:MET:HE1	2:B:604:TRP:CZ2	2.55	0.41
3:C:393:BTB:H32	3:C:393:BTB:H72	1.76	0.41
2:D:545:TYR:CZ	2:D:561:ASN:HB3	2.55	0.41
2:B:583:LEU:HB3	2:B:599:MET:CE	2.40	0.41
1:C:371:GLU:O	1:C:375:ARG:HG2	2.19	0.41
2:B:428:ASP:HA	2:B:431:ARG:HG2	2.01	0.41
1:A:155:HIS:CG	1:A:166:LEU:HD11	2.56	0.41
1:C:183:ASP:OD1	1:C:183:ASP:C	2.59	0.41
1:C:313:ASP:HA	1:C:314:PRO:HD3	1.95	0.41
1:A:113:VAL:HG13	1:A:123:VAL:HG11	2.03	0.41
2:B:599:MET:HE1	2:B:604:TRP:HZ2	1.86	0.41
1:C:61:LYS:HD2	1:C:75:THR:O	2.21	0.41
2:B:497:LEU:HA	2:B:500:LEU:HD12	2.04	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	385/394 (98%)	377 (98%)	7 (2%)	1 (0%)	41 47
1	C	389/394 (99%)	380 (98%)	9 (2%)	0	100 100
2	B	284/328 (87%)	279 (98%)	4 (1%)	1 (0%)	34 38
2	D	288/328 (88%)	282 (98%)	6 (2%)	0	100 100
All	All	1346/1444 (93%)	1318 (98%)	26 (2%)	2 (0%)	51 63

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	589	SER
1	A	387	CYS

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	319/325 (98%)	311 (98%)	8 (2%)	47 58
1	C	317/325 (98%)	308 (97%)	9 (3%)	43 53
2	B	238/264 (90%)	233 (98%)	5 (2%)	53 65
2	D	244/264 (92%)	234 (96%)	10 (4%)	30 37
All	All	1118/1178 (95%)	1086 (97%)	32 (3%)	43 52

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	LYS
1	A	36	ARG
1	A	122	ARG
1	A	177	LYS
1	A	219	LEU
1	A	264	ILE

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Mol	Chain	Res	Type
1	A	274	GLU
1	A	316	LEU
2	B	326	PHE
2	B	351	LEU
2	B	431	ARG
2	B	558	SER
2	B	589	SER
1	C	12	LYS
1	C	36	ARG
1	C	149	VAL
1	C	157	GLU
1	C	219	LEU
1	C	235	THR
1	C	264	ILE
1	C	312	LYS
1	C	371	GLU
2	D	330	ASN
2	D	370	GLU
2	D	394[A]	ARG
2	D	394[B]	ARG
2	D	462	LEU
2	D	473	GLU
2	D	536	ASN
2	D	539	GLU
2	D	562	LEU
2	D	602	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	22	ASN
1	A	32	ASN
1	A	72	ASN
1	A	308	GLN
1	A	342	HIS
2	B	364	GLN
2	B	368	HIS
2	B	552	GLN
1	C	32	ASN
1	C	72	ASN
1	C	145	GLN
1	C	261	HIS

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Mol	Chain	Res	Type
1	C	286	ASN
2	D	330	ASN
2	D	335	HIS
2	D	368	HIS
2	D	373	GLN
2	D	419	GLN
2	D	536	ASN
2	D	552	GLN
2	D	568	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues 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	$\#\|Z\|>2$
1	LLP	A	209	1	23,24,25	1.86	5 (21%)	25,32,34	1.68	5 (20%)
1	LLP	C	209	1	23,24,25	1.91	6 (26%)	25,32,34	2.26	6 (24%)

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
1	LLP	A	209	1	-	5/16/17/19	0/1/1/1
1	LLP	C	209	1	-	2/16/17/19	0/1/1/1

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	209	LLP	O3-C3	-5.87	1.23	1.37
1	C	209	LLP	O3-C3	-5.70	1.23	1.37
1	C	209	LLP	C2-N1	3.47	1.40	1.33
1	C	209	LLP	C4-C4'	3.29	1.52	1.46
1	A	209	LLP	C2-N1	3.12	1.39	1.33
1	A	209	LLP	C4-C4'	2.91	1.52	1.46
1	C	209	LLP	C4'-NZ	2.43	1.35	1.27
1	C	209	LLP	C6-N1	2.37	1.39	1.34
1	A	209	LLP	C6-N1	2.29	1.39	1.34
1	A	209	LLP	C4'-NZ	2.12	1.34	1.27
1	C	209	LLP	P-OP2	-2.01	1.47	1.54

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	209	LLP	OP4-C5'-C5	8.54	125.63	109.35
1	A	209	LLP	OP4-C5'-C5	4.95	118.78	109.35
1	C	209	LLP	C5-C6-N1	-3.41	118.15	123.82
1	A	209	LLP	CE-NZ-C4'	-3.04	109.57	118.90
1	C	209	LLP	CE-NZ-C4'	-2.69	110.66	118.90
1	A	209	LLP	C5-C6-N1	-2.62	119.45	123.82
1	C	209	LLP	C6-C5-C4	2.36	122.50	118.15
1	C	209	LLP	C2'-C2-C3	-2.29	118.06	120.89
1	C	209	LLP	C4-C4'-NZ	-2.25	113.97	124.31
1	A	209	LLP	OP4-P-OP1	-2.18	100.35	106.47
1	A	209	LLP	C4-C4'-NZ	-2.07	114.81	124.31

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	209	LLP	C4-C4'-NZ-CE
1	A	209	LLP	O-C-CA-CB
1	C	209	LLP	C4-C4'-NZ-CE
1	C	209	LLP	O-C-CA-CB
1	A	209	LLP	CA-CB-CG-CD
1	A	209	LLP	CD-CE-NZ-C4'
1	A	209	LLP	C3-C4-C4'-NZ

There are no ring outliers.

2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	209	LLP	3	0
1	C	209	LLP	4	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

1 ligand is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	BTB	C	393	-	13,13,13	0.41	0	7,16,16	0.39	0

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	BTB	C	393	-	-	6/21/21/21	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	393	BTB	C1-C2-N-C5
3	C	393	BTB	C3-C2-N-C5
3	C	393	BTB	C4-C2-N-C5
3	C	393	BTB	N-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
3	C	393	BTB	O1-C1-C2-C3
3	C	393	BTB	O1-C1-C2-C4

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	393	BTB	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	386/394 (97%)	-0.34	0 100 100	16, 26, 39, 52	0
1	C	388/394 (98%)	-0.29	1 (0%) 94 97	20, 32, 47, 57	0
2	B	289/328 (88%)	-0.29	2 (0%) 87 92	18, 28, 42, 63	0
2	D	292/328 (89%)	-0.15	1 (0%) 94 97	21, 36, 57, 73	0
All	All	1355/1444 (93%)	-0.27	4 (0%) 94 97	16, 30, 49, 73	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	443	ALA	3.2
1	C	4	HIS	2.6
2	B	590	ARG	2.3
2	B	593	ARG	2.1

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

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. 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	B-factors(Å^2)	Q<0.9
1	LLP	C	209	24/25	0.92	0.20	24,34,42,43	0
1	LLP	A	209	24/25	0.94	0.18	21,35,39,40	0

6.3 Carbohydrates

There are no monosaccharides 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. 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	B-factors(Å^2)	Q<0.9
3	BTB	C	393	14/14	0.85	0.21	59,61,61,63	0

6.5 Other polymers

There are no such residues in this entry.