Full wwPDB X-ray Structure Validation Report (i)

Sep 26, 2023 – 09:58 AM EDT

PDB ID	:	6D7Q
Title	:	Crystal Structure of Rat TRPV6*-Y466A in complex with 2-Aminoethoxydi phenyl borate (2-APB)
Authors	:	Singh, A.K.; Saotome, K.; McGoldrick, L.L.; Sobolevsky, A.I.
Deposited on	:	2018-04-25
Resolution	:	3.50 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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

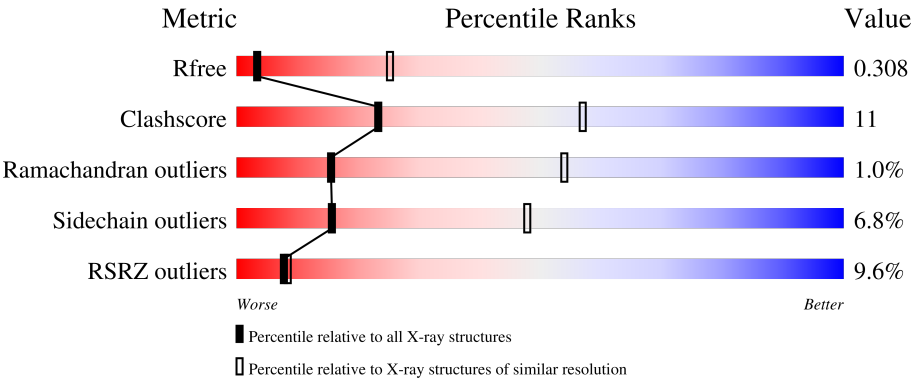
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 3.50 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))
R_{free}	130704	1659 (3.60-3.40)
Clashscore	141614	1036 (3.58-3.42)
Ramachandran outliers	138981	1005 (3.58-3.42)
Sidechain outliers	138945	1006 (3.58-3.42)
RSRZ outliers	127900	1559 (3.60-3.40)

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 of 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	672	8% 64% 20% 11%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4782 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.

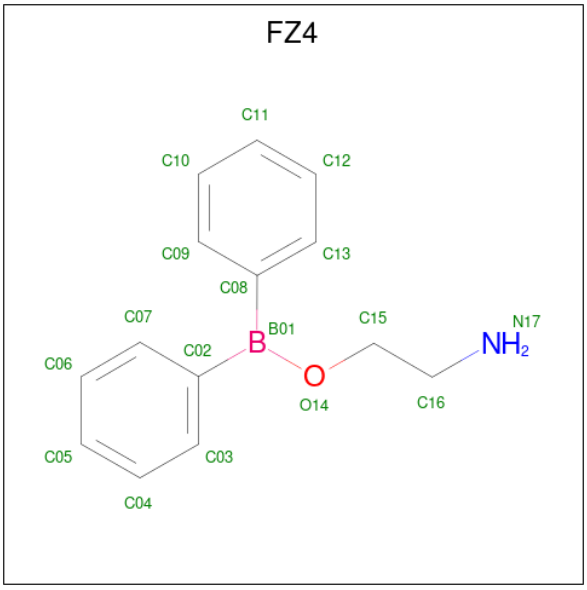
- Molecule 1 is a protein called Transient receptor potential cation channel subfamily V member 6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	596	4749	3073	796	846	34	0	0	0

There are 7 discrepancies between the modelled and reference sequences:

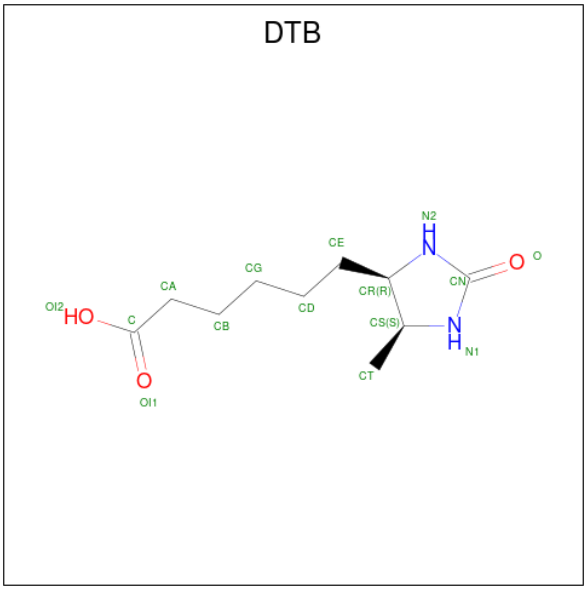
Chain	Residue	Modelled	Actual	Comment	Reference
A	62	TYR	ILE	conflict	UNP Q9R186
A	92	ASN	LEU	conflict	UNP Q9R186
A	96	GLN	MET	conflict	UNP Q9R186
A	466	ALA	TYR	engineered mutation	UNP Q9R186
A	670	VAL	-	expression tag	UNP Q9R186
A	671	PRO	-	expression tag	UNP Q9R186
A	672	ARG	-	expression tag	UNP Q9R186

- Molecule 2 is 2-aminoethyl diphenylborinate (three-letter code: FZ4) (formula: $C_{14}H_{16}BNO$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	B	C	N	O	0	0
			17	1	14	1	1		

- Molecule 3 is 6-(5-METHYL-2-OXO-IMIDAZOLIDIN-4-YL)-HEXANOIC ACID (three-letter code: DTB) (formula: $C_{10}H_{18}N_2O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			15	10	2	3		

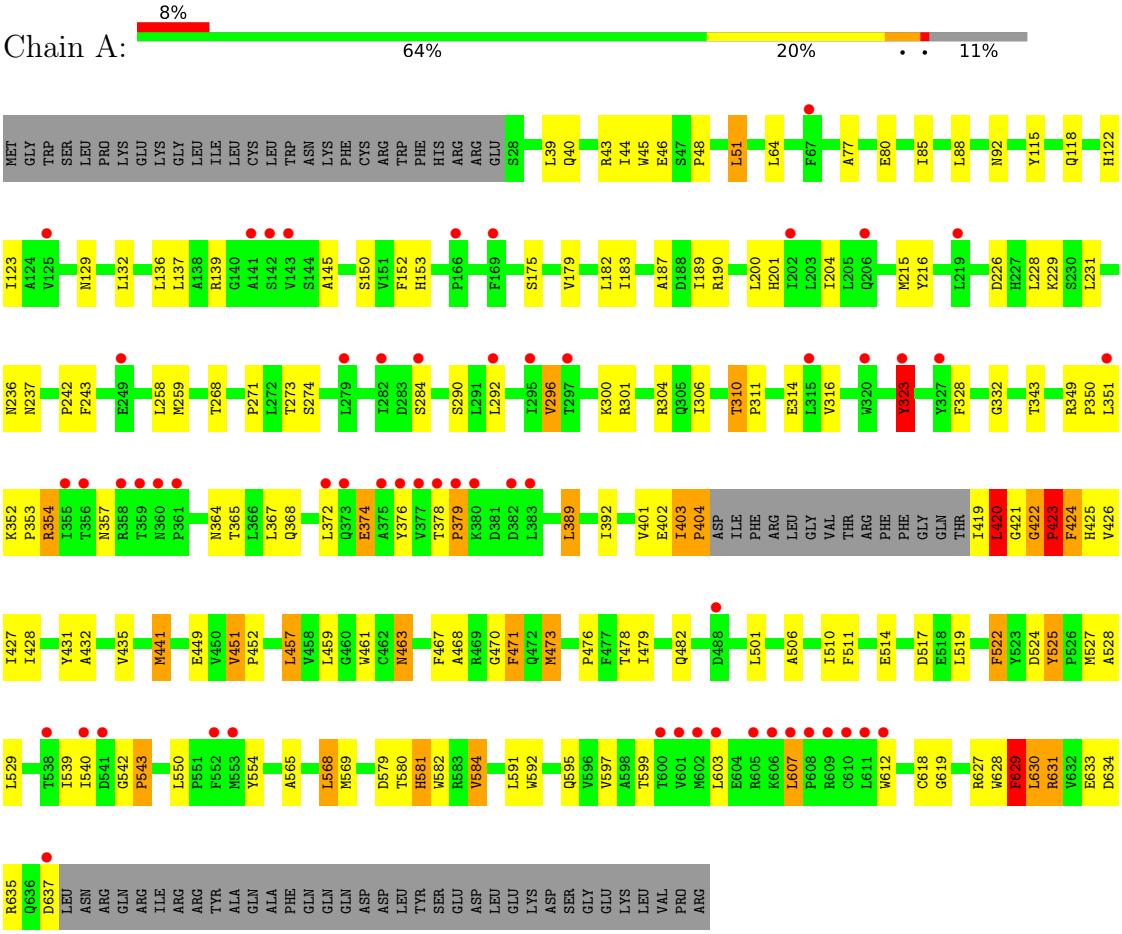
- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Ca	0	0
			1	1		

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: Transient receptor potential cation channel subfamily V member 6



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 4 21 2	Depositor
Cell constants a, b, c, α, β, γ	145.19Å 145.19Å 115.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.93 – 3.50 46.93 – 3.50	Depositor EDS
% Data completeness (in resolution range)	94.1 (46.93-3.50) 93.7 (46.93-3.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.95 (at 3.48Å)	Xtriage
Refinement program	PHENIX (1.11.1_2575: ???)	Depositor
R, R_{free}	0.275 , 0.306 0.291 , 0.308	Depositor DCC
R_{free} test set	762 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	153.4	Xtriage
Anisotropy	0.014	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 121.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.42$, $< L^2 > = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.86	EDS
Total number of atoms	4782	wwPDB-VP
Average B, all atoms (Å^2)	145.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.38% 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: CA, FZ4, DTB

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	0.31	1/4858 (0.0%)	0.62	17/6601 (0.3%)

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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	629	PHE	C-N	-12.31	1.05	1.34

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	629	PHE	O-C-N	-16.15	96.87	122.70
1	A	629	PHE	CA-C-N	10.33	139.93	117.20
1	A	629	PHE	CB-CA-C	-9.93	90.54	110.40
1	A	629	PHE	N-CA-C	9.36	136.27	111.00
1	A	404	PRO	CA-N-CD	-8.50	99.60	111.50
1	A	630	LEU	N-CA-C	8.16	133.02	111.00
1	A	582	TRP	N-CA-C	7.57	131.44	111.00
1	A	630	LEU	N-CA-CB	-7.15	96.11	110.40
1	A	581	HIS	CB-CA-C	-7.14	96.12	110.40
1	A	582	TRP	N-CA-CB	-7.07	97.87	110.60
1	A	354	ARG	N-CA-C	6.96	129.78	111.00
1	A	323	TYR	CB-CA-C	-6.78	96.85	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	471	PHE	N-CA-C	-6.51	93.41	111.00
1	A	457	LEU	CA-CB-CG	5.74	128.49	115.30
1	A	357	ASN	N-CA-C	5.34	125.42	111.00
1	A	637	ASP	CB-CG-OD2	5.19	122.97	118.30
1	A	420	LEU	CA-CB-CG	5.09	127.01	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	629	PHE	Mainchain

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	4749	0	4779	106	0
2	A	17	0	0	1	0
3	A	15	0	17	1	0
4	A	1	0	0	0	0
All	All	4782	0	4796	108	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 11.

All (108) 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:473:MET:O	1:A:476:PRO:HD2	1.65	0.94
1:A:374:GLU:HB2	1:A:376:TYR:HD2	1.35	0.88
1:A:323:TYR:O	1:A:612:TRP:CZ3	2.33	0.82
1:A:354:ARG:O	1:A:354:ARG:HG2	1.80	0.80
1:A:403:ILE:N	1:A:404:PRO:HD3	2.03	0.73
1:A:420:LEU:HD13	1:A:421:GLY:H	1.54	0.73
1:A:374:GLU:CB	1:A:376:TYR:HD2	2.03	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:451:VAL:HG13	1:A:452:PRO:HD3	1.74	0.69
1:A:522:PHE:HB3	1:A:528:ALA:HA	1.78	0.66
1:A:374:GLU:HB2	1:A:376:TYR:CD2	2.26	0.65
1:A:374:GLU:CB	1:A:376:TYR:CD2	2.83	0.62
1:A:403:ILE:N	1:A:404:PRO:CD	2.63	0.61
1:A:422:GLY:O	1:A:424:PHE:N	2.34	0.61
1:A:540:ILE:HG22	1:A:542:GLY:H	1.66	0.60
1:A:354:ARG:HB2	1:A:368:GLN:HA	1.86	0.57
1:A:619:GLY:N	1:A:627:ARG:O	2.34	0.57
1:A:470:GLY:H	1:A:592:TRP:HE1	1.51	0.57
1:A:183:ILE:HD13	1:A:187:ALA:HB3	1.87	0.56
1:A:424:PHE:O	1:A:463:ASN:ND2	2.28	0.56
1:A:473:MET:C	1:A:476:PRO:HD2	2.26	0.56
1:A:422:GLY:H	1:A:423:PRO:CD	2.19	0.56
1:A:43:ARG:NH1	1:A:46:GLU:OE1	2.39	0.56
1:A:271:PRO:HB2	1:A:635:ARG:HG3	1.89	0.54
1:A:45:TRP:HA	1:A:51:LEU:HG	1.90	0.54
1:A:92:ASN:OD1	1:A:129:ASN:ND2	2.41	0.53
1:A:402:GLU:C	1:A:404:PRO:CD	2.78	0.53
1:A:296:VAL:HG23	1:A:420:LEU:HD11	1.90	0.52
1:A:354:ARG:O	1:A:354:ARG:CG	2.48	0.52
1:A:401:VAL:HG23	1:A:402:GLU:HG2	1.93	0.51
1:A:479:ILE:HA	1:A:482:GLN:HB3	1.93	0.50
2:A:701:FZ4:C15	2:A:701:FZ4:C02	2.90	0.50
1:A:470:GLY:O	1:A:471:PHE:C	2.50	0.50
1:A:243:PHE:HA	1:A:258:LEU:HD13	1.93	0.49
1:A:519:LEU:HD21	1:A:543:PRO:HB3	1.94	0.49
1:A:580:THR:C	1:A:581:HIS:O	2.49	0.49
1:A:343:THR:HG21	1:A:461:TRP:HE1	1.77	0.49
1:A:316:VAL:HG21	1:A:597:VAL:HG13	1.95	0.49
1:A:179:VAL:HG21	1:A:215:MET:SD	2.53	0.48
1:A:511:PHE:HA	1:A:514:GLU:HG2	1.94	0.48
1:A:581:HIS:O	1:A:584:VAL:HG23	2.14	0.48
1:A:402:GLU:C	1:A:404:PRO:HD3	2.34	0.48
1:A:389:LEU:HA	1:A:392:ILE:HG22	1.96	0.48
1:A:190:ARG:NH2	1:A:229:LYS:O	2.46	0.47
1:A:236:ASN:OD1	1:A:237:ASN:N	2.47	0.47
1:A:378:THR:N	1:A:379:PRO:HD2	2.29	0.47
1:A:122:HIS:HE1	1:A:145:ALA:HB3	1.79	0.47
1:A:115:TYR:HA	1:A:152:PHE:HE1	1.81	0.46
1:A:201:HIS:HA	1:A:204:ILE:HD12	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:328:PHE:HE2	1:A:599:THR:HG21	1.79	0.46
1:A:421:GLY:HA3	1:A:595:GLN:HG3	1.97	0.46
1:A:506:ALA:O	1:A:510:ILE:HG12	2.16	0.46
1:A:150:SER:HA	1:A:153:HIS:NE2	2.30	0.46
1:A:468:ALA:HB3	1:A:478:THR:HG21	1.97	0.46
1:A:618:CYS:HA	1:A:628:TRP:HA	1.97	0.45
1:A:226:ASP:N	1:A:226:ASP:OD1	2.50	0.45
1:A:423:PRO:O	1:A:426:VAL:HG12	2.17	0.45
1:A:175:SER:O	1:A:179:VAL:HG23	2.16	0.45
1:A:200:LEU:HB3	1:A:216:TYR:HE1	1.82	0.45
1:A:543:PRO:HB2	1:A:554:TYR:CZ	2.52	0.45
1:A:80:GLU:HG3	1:A:85:ILE:HD11	1.99	0.45
3:A:702:DTB:HCG1	3:A:702:DTB:HCR	1.75	0.45
1:A:425:HIS:HA	1:A:428:ILE:HG22	1.98	0.45
1:A:579:ASP:HA	1:A:584:VAL:HG11	1.99	0.45
1:A:374:GLU:HB3	1:A:376:TYR:CD2	2.53	0.44
1:A:48:PRO:HB2	1:A:64:LEU:HD21	1.99	0.44
1:A:522:PHE:CB	1:A:528:ALA:HA	2.48	0.44
1:A:603:LEU:O	1:A:607:LEU:N	2.51	0.44
1:A:137:LEU:HD21	1:A:182:LEU:HD23	1.98	0.44
1:A:350:PRO:HB3	1:A:372:LEU:HB2	2.00	0.43
1:A:441:MET:HG2	1:A:449:GLU:HA	2.00	0.43
1:A:422:GLY:H	1:A:423:PRO:HD2	1.82	0.43
1:A:423:PRO:O	1:A:425:HIS:N	2.52	0.43
1:A:519:LEU:HD11	1:A:543:PRO:HB3	1.99	0.43
1:A:332:GLY:HA2	1:A:467:PHE:CZ	2.54	0.43
1:A:421:GLY:HA2	1:A:595:GLN:HE21	1.83	0.43
1:A:189:ILE:HD12	1:A:231:LEU:HD22	2.00	0.43
1:A:627:ARG:HB2	1:A:629:PHE:CE2	2.54	0.42
1:A:634:ASP:OD1	1:A:634:ASP:N	2.52	0.42
1:A:274:SER:HA	1:A:633:GLU:HA	2.01	0.42
1:A:568:LEU:HD13	1:A:568:LEU:HA	1.82	0.42
1:A:631:ARG:HH11	1:A:631:ARG:HB3	1.84	0.42
1:A:301:ARG:O	1:A:304:ARG:NH1	2.41	0.42
1:A:150:SER:HA	1:A:153:HIS:CD2	2.55	0.42
1:A:432:ALA:HA	1:A:435:VAL:HG22	2.01	0.42
1:A:374:GLU:HB3	1:A:376:TYR:CE2	2.54	0.42
1:A:310:THR:HG23	1:A:311:PRO:HD3	2.00	0.42
1:A:118:GLN:NE2	1:A:123:ILE:HG12	2.35	0.42
1:A:306:ILE:HD13	1:A:306:ILE:HA	1.92	0.42
1:A:259:MET:HE3	1:A:311:PRO:HG3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:201:HIS:CE1	1:A:242:PRO:HD3	2.55	0.42
1:A:296:VAL:O	1:A:420:LEU:HG	2.19	0.41
1:A:427:ILE:CG2	1:A:459:LEU:HB3	2.51	0.41
1:A:40:GLN:O	1:A:44:ILE:HG12	2.20	0.41
1:A:132:LEU:O	1:A:136:LEU:N	2.49	0.41
1:A:354:ARG:HH12	1:A:365:THR:HG21	1.86	0.41
1:A:284:SER:HA	1:A:290:SER:HB2	2.01	0.41
1:A:292:LEU:O	1:A:296:VAL:HG12	2.21	0.41
1:A:524:ASP:O	1:A:528:ALA:N	2.54	0.41
1:A:365:THR:HG23	1:A:367:LEU:HD13	2.02	0.41
1:A:268:THR:HG22	1:A:273:THR:HG23	2.02	0.41
1:A:352:LYS:HA	1:A:353:PRO:HD3	1.90	0.41
1:A:419:ILE:O	1:A:420:LEU:C	2.58	0.41
1:A:525:TYR:O	1:A:529:LEU:HG	2.21	0.41
1:A:40:GLN:HA	1:A:77:ALA:HB3	2.03	0.40
1:A:420:LEU:CD1	1:A:421:GLY:H	2.28	0.40
1:A:565:ALA:O	1:A:569:MET:HG2	2.21	0.40
1:A:300:LYS:HD3	1:A:300:LYS:HA	1.87	0.40
1:A:43:ARG:HA	1:A:43:ARG:HD3	1.90	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	592/672 (88%)	535 (90%)	51 (9%)	6 (1%)	15 54

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	423	PRO
1	A	424	PHE

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Mol	Chain	Res	Type
1	A	323	TYR
1	A	379	PRO
1	A	422	GLY
1	A	543	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	512/583 (88%)	477 (93%)	35 (7%)	16 48

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	LEU
1	A	51	LEU
1	A	88	LEU
1	A	139	ARG
1	A	228	LEU
1	A	296	VAL
1	A	310	THR
1	A	314	GLU
1	A	349	ARG
1	A	351	LEU
1	A	364	ASN
1	A	374	GLU
1	A	389	LEU
1	A	403	ILE
1	A	420	LEU
1	A	423	PRO
1	A	431	TYR
1	A	441	MET
1	A	451	VAL
1	A	457	LEU
1	A	463	ASN
1	A	473	MET

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Mol	Chain	Res	Type
1	A	501	LEU
1	A	517	ASP
1	A	522	PHE
1	A	525	TYR
1	A	527	MET
1	A	539	ILE
1	A	550	LEU
1	A	568	LEU
1	A	584	VAL
1	A	591	LEU
1	A	607	LEU
1	A	630	LEU
1	A	631	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	128	GLN
1	A	482	GLN
1	A	595	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 monosaccharides 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	$\#\|Z\| > 2$
2	FZ4	A	701	-	16,18,18	0.62	0	17,22,22	1.53	3 (17%)
3	DTB	A	702	-	15,15,15	3.06	3 (20%)	16,19,19	2.39	5 (31%)

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
2	FZ4	A	701	-	-	5/12/12/12	0/2/2/2
3	DTB	A	702	-	-	1/8/20/20	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	702	DTB	CN-N2	8.04	1.48	1.35
3	A	702	DTB	CN-N1	7.91	1.48	1.35
3	A	702	DTB	O-CN	-2.06	1.19	1.23

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	702	DTB	CR-CS-N1	4.81	108.30	102.43
3	A	702	DTB	CS-CR-N2	4.29	107.54	102.17
3	A	702	DTB	CS-N1-CN	-4.10	107.89	112.42
2	A	701	FZ4	C07-C02-C03	3.30	120.57	116.88
3	A	702	DTB	CR-N2-CN	-3.29	108.18	112.46
2	A	701	FZ4	C13-C08-C09	3.04	120.28	116.88
3	A	702	DTB	CT-CS-N1	-2.73	108.45	111.70
2	A	701	FZ4	C06-C07-C02	-2.10	119.49	121.57

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	701	FZ4	C08-B01-O14-C15
2	A	701	FZ4	O14-C15-C16-N17
3	A	702	DTB	CE-CD-CG-CB
2	A	701	FZ4	O14-B01-C02-C03
2	A	701	FZ4	O14-B01-C02-C07
2	A	701	FZ4	C08-B01-C02-C07

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	701	FZ4	1	0
3	A	702	DTB	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	629:PHE	C	630:LEU	N	1.05

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	596/672 (88%)	0.57	57 (9%)	8	8	87, 139, 197, 239	0

All (57) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	351	LEU	7.4
1	A	612	TRP	7.3
1	A	610	CYS	6.6
1	A	373	GLN	5.5
1	A	372	LEU	5.4
1	A	602	MET	5.3
1	A	360	ASN	5.2
1	A	292	LEU	5.2
1	A	382	ASP	5.0
1	A	607	LEU	4.8
1	A	600	THR	4.6
1	A	608	PRO	4.6
1	A	379	PRO	4.6
1	A	611	LEU	4.4
1	A	380	LYS	4.2
1	A	606	LYS	4.0
1	A	376	TYR	4.0
1	A	377	VAL	3.9
1	A	637	ASP	3.7
1	A	143	VAL	3.6
1	A	323	TYR	3.6
1	A	378	THR	3.5
1	A	375	ALA	3.5
1	A	359	THR	3.3
1	A	284	SER	3.3
1	A	538	THR	3.1
1	A	327	TYR	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	361	PRO	3.1
1	A	166	PRO	3.1
1	A	142	SER	3.1
1	A	540	ILE	3.0
1	A	553	MET	3.0
1	A	603	LEU	2.9
1	A	206	GLN	2.6
1	A	356	THR	2.6
1	A	605	ARG	2.6
1	A	315	LEU	2.6
1	A	169	PHE	2.5
1	A	249	GLU	2.5
1	A	552	PHE	2.5
1	A	295	ILE	2.4
1	A	609	ARG	2.4
1	A	279	LEU	2.4
1	A	601	VAL	2.4
1	A	282	ILE	2.4
1	A	320	TRP	2.3
1	A	541	ASP	2.3
1	A	383	LEU	2.2
1	A	67	PHE	2.2
1	A	219	LEU	2.2
1	A	202	ILE	2.2
1	A	297	THR	2.1
1	A	141	ALA	2.1
1	A	358	ARG	2.1
1	A	355	ILE	2.1
1	A	488	ASP	2.1
1	A	125	VAL	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 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
4	CA	A	703	1/1	0.21	0.25	116,116,116,116	1
2	FZ4	A	701	17/17	0.84	0.55	98,109,116,119	0
3	DTB	A	702	15/15	0.85	0.43	92,111,140,151	0

6.5 Other polymers

There are no such residues in this entry.