



Full wwPDB X-ray Structure Validation Report ⓘ

May 24, 2020 – 12:44 am BST

PDB ID : 4DX1
Title : Crystal structure of the human TRPV4 ankyrin repeat domain
Authors : Inada, H.; Gaudet, R.
Deposited on : 2012-02-27
Resolution : 2.85 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 : 2.11
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) : 2.11

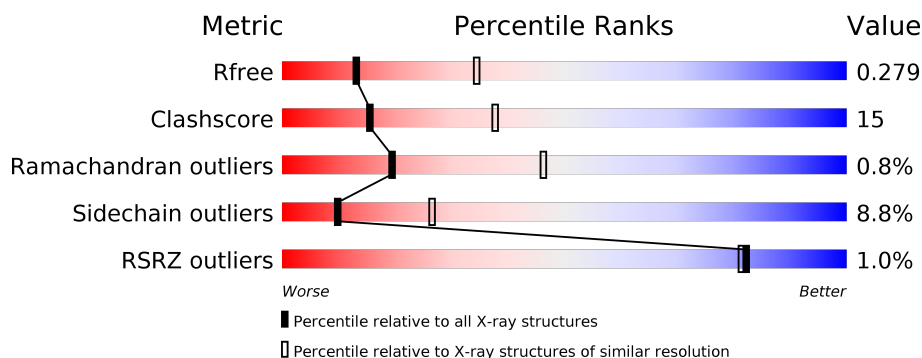
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.85 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	3168 (2.90-2.82)
Clashscore	141614	3438 (2.90-2.82)
Ramachandran outliers	138981	3348 (2.90-2.82)
Sidechain outliers	138945	3351 (2.90-2.82)
RSRZ outliers	127900	3103 (2.90-2.82)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	259	<div> <div style="width: 2%;"></div> <div style="width: 64%; background-color: green;"></div> <div style="width: 27%; background-color: yellow;"></div> <div style="width: 6%; background-color: orange;"></div> <div style="width: 3%; background-color: red;"></div> <div style="width: 2%; background-color: grey;"></div> </div> <div> <div style="width: 2%; background-color: red;"></div> <div style="width: 65%; background-color: green;"></div> <div style="width: 27%; background-color: yellow;"></div> <div style="width: 6%; background-color: orange;"></div> <div style="width: 2%; background-color: grey;"></div> </div>
1	B	259	<div> <div style="width: 2%;"></div> <div style="width: 65%; background-color: green;"></div> <div style="width: 27%; background-color: yellow;"></div> <div style="width: 6%; background-color: orange;"></div> <div style="width: 3%; background-color: red;"></div> <div style="width: 2%; background-color: grey;"></div> </div> <div> <div style="width: 2%; background-color: red;"></div> <div style="width: 65%; background-color: green;"></div> <div style="width: 27%; background-color: yellow;"></div> <div style="width: 6%; background-color: orange;"></div> <div style="width: 2%; background-color: grey;"></div> </div>

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
2	PO4	B	502	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4029 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 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	250	Total	C	N	O	S	0	0	0
			1995	1260	361	364	10			
1	B	249	Total	C	N	O	S	0	0	0
			1986	1255	360	361	10			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	148	MET	-	INITIATING METHIONINE	UNP Q9HBA0
A	398	ALA	-	EXPRESSION TAG	UNP Q9HBA0
A	399	ALA	-	EXPRESSION TAG	UNP Q9HBA0
A	400	ALA	-	EXPRESSION TAG	UNP Q9HBA0
A	401	HIS	-	EXPRESSION TAG	UNP Q9HBA0
A	402	HIS	-	EXPRESSION TAG	UNP Q9HBA0
A	403	HIS	-	EXPRESSION TAG	UNP Q9HBA0
A	404	HIS	-	EXPRESSION TAG	UNP Q9HBA0
A	405	HIS	-	EXPRESSION TAG	UNP Q9HBA0
A	406	HIS	-	EXPRESSION TAG	UNP Q9HBA0
B	148	MET	-	INITIATING METHIONINE	UNP Q9HBA0
B	398	ALA	-	EXPRESSION TAG	UNP Q9HBA0
B	399	ALA	-	EXPRESSION TAG	UNP Q9HBA0
B	400	ALA	-	EXPRESSION TAG	UNP Q9HBA0
B	401	HIS	-	EXPRESSION TAG	UNP Q9HBA0
B	402	HIS	-	EXPRESSION TAG	UNP Q9HBA0
B	403	HIS	-	EXPRESSION TAG	UNP Q9HBA0
B	404	HIS	-	EXPRESSION TAG	UNP Q9HBA0
B	405	HIS	-	EXPRESSION TAG	UNP Q9HBA0
B	406	HIS	-	EXPRESSION TAG	UNP Q9HBA0

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	P	0	0
			5	4	1		
2	A	1	Total	O	P	0	0
			5	4	1		
2	B	1	Total	O	P	0	0
			5	4	1		
2	B	1	Total	O	P	0	0
			5	4	1		
2	B	1	Total	O	P	0	0
			5	4	1		

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



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

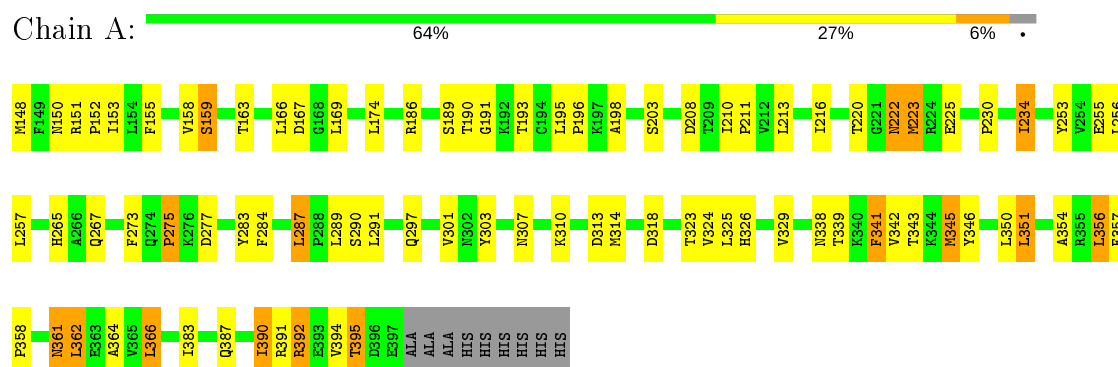
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	10	Total	O	0	0
			10	10		
4	B	7	Total	O	0	0
			7	7		

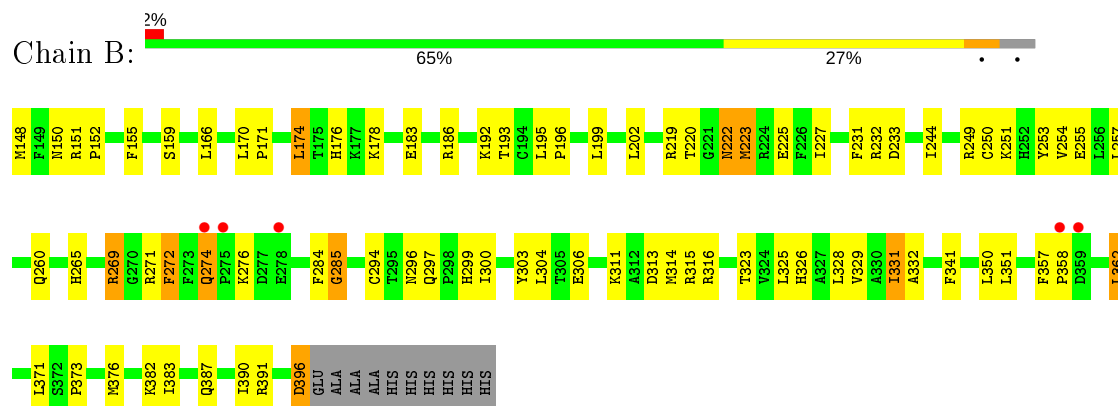
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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 4



- Molecule 1: Transient receptor potential cation channel subfamily V member 4



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	53.37Å 53.37Å 440.71Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	39.12 – 2.85 39.12 – 2.85	Depositor EDS
% Data completeness (in resolution range)	99.6 (39.12-2.85) 99.6 (39.12-2.85)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.31 (at 2.86Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.215 , 0.279 0.214 , 0.279	Depositor DCC
R_{free} test set	930 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å ²)	76.6	Xtriage
Anisotropy	0.062	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 44.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.050 for -h,-k,l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	4029	wwPDB-VP
Average B, all atoms (Å ²)	81.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.16% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, PO4

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	0.60	0/2034	0.73	0/2748
1	B	0.63	0/2025	0.77	1/2736 (0.0%)
All	All	0.62	0/4059	0.75	1/5484 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	285	GLY	N-CA-C	-5.20	100.11	113.10

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	1995	0	2007	60	0
1	B	1986	0	2001	59	1
2	A	10	0	0	0	0
2	B	15	0	0	1	0
3	A	6	0	8	0	0
4	A	10	0	0	0	0
4	B	7	0	0	2	0
All	All	4029	0	4016	119	1

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 15.

All (119) 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:B:269:ARG:HH11	1:B:269:ARG:HG2	1.14	1.12
1:B:231:PHE:CZ	1:B:244:ILE:HD11	2.03	0.94
1:B:274:GLN:N	1:B:274:GLN:HE21	1.66	0.93
1:A:383:ILE:HG22	1:A:387:GLN:NE2	1.91	0.85
1:B:269:ARG:HH11	1:B:269:ARG:CG	1.92	0.82
1:B:231:PHE:HZ	1:B:244:ILE:HD11	1.43	0.80
1:A:383:ILE:HG22	1:A:387:GLN:HE21	1.48	0.79
1:B:265:HIS:HE1	1:B:313:ASP:H	1.38	0.72
1:B:265:HIS:CE1	1:B:313:ASP:H	2.08	0.71
1:B:269:ARG:NH1	1:B:269:ARG:HG2	1.91	0.68
1:A:222:ASN:C	1:A:222:ASN:HD22	1.95	0.68
1:A:392:ARG:HH11	1:A:392:ARG:HG3	1.62	0.65
1:B:357:PHE:HB3	4:B:603:HOH:O	1.95	0.65
1:B:250:CYS:HG	1:B:253:TYR:HD2	1.45	0.64
1:A:151:ARG:HB3	1:A:152:PRO:HD3	1.79	0.64
1:B:151:ARG:HB3	1:B:152:PRO:HD3	1.80	0.63
1:A:394:VAL:HG13	1:A:395:THR:N	2.13	0.63
1:A:195:LEU:HB3	1:A:196:PRO:CD	2.28	0.63
1:A:195:LEU:HB3	1:A:196:PRO:HD3	1.81	0.62
1:B:383:ILE:HB	1:B:387:GLN:NE2	2.14	0.62
1:A:150:ASN:OD1	1:A:153:ILE:HG13	2.00	0.61
1:B:300:ILE:HG22	1:B:304:LEU:HD12	1.83	0.61
1:B:323:THR:H	1:B:326:HIS:HD2	1.49	0.60
1:B:328:LEU:HA	1:B:331:ILE:HD11	1.84	0.60
1:B:396:ASP:OD1	1:B:396:ASP:N	2.35	0.60
1:A:265:HIS:HE1	1:A:313:ASP:H	1.49	0.59
1:A:265:HIS:CE1	1:A:313:ASP:H	2.20	0.59
1:B:255:GLU:HG2	1:B:303:TYR:CE1	2.38	0.58
1:A:325:LEU:HD11	1:A:362:LEU:HD13	1.85	0.58
1:A:323:THR:H	1:A:326:HIS:CD2	2.22	0.58
1:A:364:ALA:O	1:A:366:LEU:HD13	2.04	0.57
1:A:267:GLN:HG3	1:A:287:LEU:HD23	1.86	0.57
1:B:326:HIS:HB3	1:B:376:MET:HE1	1.87	0.57
1:B:155:PHE:O	1:B:159:SER:HB2	2.05	0.57
1:B:222:ASN:ND2	1:B:225:GLU:H	2.02	0.57
1:A:391:ARG:O	1:A:395:THR:HB	2.05	0.56
1:A:174:LEU:CD1	1:A:220:THR:HG22	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:325:LEU:HB3	1:A:346:TYR:CE2	2.41	0.56
1:A:351:LEU:O	1:A:354:ALA:HB3	2.06	0.55
1:B:300:ILE:CG2	1:B:304:LEU:HD12	2.37	0.55
1:B:315:ARG:HA	1:B:362:LEU:HD21	1.89	0.54
1:A:155:PHE:O	1:A:159:SER:HB2	2.08	0.53
1:A:394:VAL:CG1	1:A:395:THR:N	2.72	0.53
1:B:195:LEU:HB3	1:B:196:PRO:HD3	1.90	0.53
1:A:392:ARG:NH1	1:A:392:ARG:HG3	2.24	0.52
1:B:265:HIS:HE1	1:B:313:ASP:N	2.07	0.52
1:B:294:CYS:SG	1:B:331:ILE:HG12	2.49	0.52
1:A:345:MET:CE	1:A:345:MET:HA	2.39	0.52
1:A:253:TYR:O	1:A:257:LEU:HG	2.10	0.52
1:B:150:ASN:O	1:B:151:ARG:C	2.48	0.52
1:A:163:THR:HA	1:A:166:LEU:HD12	1.90	0.52
1:A:166:LEU:O	1:A:167:ASP:C	2.49	0.51
1:B:232:ARG:NH1	4:B:604:HOH:O	2.43	0.51
1:B:249:ARG:HA	1:B:297:GLN:HE22	1.76	0.51
1:B:250:CYS:O	1:B:254:VAL:HG23	2.10	0.51
1:B:326:HIS:HE1	1:B:371:LEU:O	1.93	0.51
1:A:158:VAL:HG11	1:A:213:LEU:HD11	1.92	0.51
1:A:290:SER:HA	1:A:324:VAL:HG23	1.94	0.50
1:A:186:ARG:NH2	1:A:230:PRO:HD2	2.25	0.50
1:B:223:MET:O	1:B:227:ILE:HG13	2.11	0.50
1:A:297:GLN:O	1:A:301:VAL:HG23	2.11	0.50
1:A:310:LYS:HZ2	1:A:310:LYS:HB3	1.77	0.50
1:A:222:ASN:HD22	1:A:223:MET:N	2.08	0.50
1:B:332:ALA:O	1:B:382:LYS:HD2	2.12	0.49
1:B:250:CYS:SG	1:B:253:TYR:HD2	2.34	0.49
1:B:174:LEU:CD1	1:B:220:THR:HG22	2.43	0.49
1:B:193:THR:O	1:B:196:PRO:HD2	2.12	0.49
1:A:394:VAL:CG1	1:A:395:THR:H	2.25	0.49
1:A:210:ILE:HB	1:A:211:PRO:HD3	1.96	0.48
1:A:323:THR:H	1:A:326:HIS:HD2	1.60	0.48
1:A:338:ASN:O	1:A:342:VAL:HG23	2.13	0.48
1:B:299:HIS:CD2	2:B:503:PO4:O1	2.67	0.48
1:A:222:ASN:ND2	1:A:222:ASN:C	2.66	0.48
1:A:283:TYR:OH	1:A:318:ASP:OD2	2.26	0.48
1:B:323:THR:H	1:B:326:HIS:CD2	2.32	0.48
1:A:255:GLU:HA	1:A:303:TYR:CE2	2.50	0.47
1:A:361:ASN:HD22	1:A:362:LEU:N	2.12	0.47
1:A:265:HIS:HE1	1:A:313:ASP:N	2.12	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:274:GLN:H	1:B:274:GLN:HE21	1.54	0.46
1:A:190:THR:OG1	1:A:191:GLY:N	2.48	0.46
1:B:170:LEU:N	1:B:171:PRO:HD2	2.31	0.46
1:A:284:PHE:CE1	1:A:291:LEU:HB2	2.51	0.46
1:A:222:ASN:ND2	1:A:225:GLU:H	2.15	0.45
1:A:394:VAL:HG13	1:A:395:THR:H	1.79	0.45
1:B:227:ILE:HG23	1:B:257:LEU:HD22	1.99	0.45
1:B:272:PHE:CD1	1:B:272:PHE:N	2.84	0.45
1:B:199:LEU:HA	1:B:202:LEU:HD21	1.99	0.44
1:A:275:PRO:C	1:A:277:ASP:H	2.19	0.44
1:A:341:PHE:CD2	1:A:341:PHE:C	2.91	0.44
1:B:326:HIS:CE1	1:B:373:PRO:HD3	2.53	0.43
1:A:339:THR:O	1:A:343:THR:HG23	2.18	0.43
1:B:186:ARG:HA	1:B:192:LYS:O	2.19	0.43
1:A:390:ILE:HG22	1:A:391:ARG:N	2.34	0.43
1:A:169:LEU:HD23	1:A:216:ILE:HD13	2.01	0.43
1:B:325:LEU:O	1:B:329:VAL:HG23	2.18	0.42
1:B:269:ARG:NH1	1:B:269:ARG:CG	2.61	0.42
1:A:193:THR:OG1	1:A:196:PRO:HD2	2.18	0.42
1:B:314:MET:C	1:B:316:ARG:H	2.22	0.42
1:A:151:ARG:O	1:A:152:PRO:C	2.56	0.42
1:A:158:VAL:HB	1:A:198:ALA:HB2	2.00	0.42
1:B:357:PHE:HA	1:B:358:PRO:HD3	1.91	0.42
1:A:234:ILE:H	1:A:234:ILE:HG12	1.61	0.42
1:B:176:HIS:O	1:B:178:LYS:HG3	2.19	0.42
1:B:331:ILE:HG13	1:B:331:ILE:H	1.53	0.41
1:B:166:LEU:HA	1:B:166:LEU:HD23	1.73	0.41
1:B:232:ARG:HD2	1:B:271:ARG:NH1	2.36	0.41
1:B:274:GLN:CA	1:B:274:GLN:HE21	2.27	0.41
1:A:357:PHE:HA	1:A:358:PRO:HD3	1.86	0.41
1:A:387:GLN:HB3	1:A:391:ARG:HH21	1.86	0.41
1:A:310:LYS:NZ	1:A:310:LYS:HB3	2.36	0.41
1:B:326:HIS:CE1	1:B:371:LEU:O	2.74	0.41
1:A:314:MET:HE1	1:A:356:LEU:HD13	2.02	0.41
1:A:289:LEU:HD11	1:A:301:VAL:HG13	2.02	0.41
1:B:383:ILE:HB	1:B:387:GLN:HE22	1.82	0.41
1:A:325:LEU:O	1:A:329:VAL:HG23	2.21	0.40
1:B:306:GLU:HA	1:B:311:LYS:HE2	2.03	0.40
1:B:284:PHE:C	1:B:285:GLY:O	2.58	0.40
1:B:151:ARG:O	1:B:152:PRO:C	2.58	0.40
1:B:390:ILE:HG22	1:B:391:ARG:N	2.37	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:219:ARG:NH2	1:B:233:ASP:OD2[5_664]	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	248/259 (96%)	217 (88%)	28 (11%)	3 (1%)	13	35
1	B	247/259 (95%)	219 (89%)	27 (11%)	1 (0%)	34	62
All	All	495/518 (96%)	436 (88%)	55 (11%)	4 (1%)	19	46

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	273	PHE
1	B	251	LYS
1	A	208	ASP
1	A	275	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	216/222 (97%)	195 (90%)	21 (10%)	8	22
1	B	215/222 (97%)	198 (92%)	17 (8%)	12	31

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	431/444 (97%)	393 (91%)	38 (9%)	10	26

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

Mol	Chain	Res	Type
1	A	148	MET
1	A	159	SER
1	A	189	SER
1	A	203	SER
1	A	222	ASN
1	A	223	MET
1	A	234	ILE
1	A	256	LEU
1	A	287	LEU
1	A	307	ASN
1	A	341	PHE
1	A	345	MET
1	A	350	LEU
1	A	351	LEU
1	A	356	LEU
1	A	361	ASN
1	A	362	LEU
1	A	366	LEU
1	A	390	ILE
1	A	392	ARG
1	A	395	THR
1	B	148	MET
1	B	174	LEU
1	B	183	GLU
1	B	222	ASN
1	B	223	MET
1	B	260	GLN
1	B	269	ARG
1	B	272	PHE
1	B	274	GLN
1	B	276	LYS
1	B	296	ASN
1	B	331	ILE
1	B	341	PHE
1	B	350	LEU
1	B	351	LEU
1	B	362	LEU

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Mol	Chain	Res	Type
1	B	396	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	222	ASN
1	A	239	GLN
1	A	265	HIS
1	A	296	ASN
1	A	326	HIS
1	A	361	ASN
1	A	368	ASN
1	A	387	GLN
1	B	222	ASN
1	B	265	HIS
1	B	274	GLN
1	B	296	ASN
1	B	297	GLN
1	B	326	HIS
1	B	361	ASN
1	B	368	ASN
1	B	387	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](#)

6 ligands 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	$\# Z > 2$
2	PO4	B	503	-	4,4,4	0.71	0	6,6,6	0.68	0
2	PO4	B	501	-	4,4,4	0.91	0	6,6,6	0.73	0
2	PO4	A	501	-	4,4,4	0.86	0	6,6,6	0.52	0
2	PO4	A	502	-	4,4,4	0.80	0	6,6,6	0.53	0
2	PO4	B	502	-	4,4,4	0.84	0	6,6,6	0.62	0
3	GOL	A	503	-	5,5,5	0.48	0	5,5,5	0.65	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	GOL	A	503	-	-	4/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	503	GOL	O1-C1-C2-C3
3	A	503	GOL	C1-C2-C3-O3
3	A	503	GOL	O1-C1-C2-O2
3	A	503	GOL	O2-C2-C3-O3

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	503	PO4	1	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	250/259 (96%)	-0.38	0 100 100	54, 76, 112, 149	0
1	B	249/259 (96%)	-0.35	5 (2%) 65 62	59, 78, 104, 126	0
All	All	499/518 (96%)	-0.36	5 (1%) 82 81	54, 77, 108, 149	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	358	PRO	3.5
1	B	359	ASP	2.7
1	B	274	GLN	2.4
1	B	275	PRO	2.3
1	B	278	GLU	2.2

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. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	PO4	B	502	5/5	0.74	0.42	183,183,184,184	0
3	GOL	A	503	6/6	0.76	0.18	101,103,104,104	0
2	PO4	B	503	5/5	0.91	0.24	130,130,131,131	0
2	PO4	A	502	5/5	0.95	0.13	116,117,117,117	0
2	PO4	B	501	5/5	0.98	0.07	71,71,72,73	0
2	PO4	A	501	5/5	0.99	0.10	63,64,65,66	0

6.5 Other polymers [i](#)

There are no such residues in this entry.