



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:08 PM GMT

PDB ID : 3W9F
Title : Crystal structure of the ankilin repeat domain of chicken TRPV4 in complex with IP3
Authors : Itoh, Y.; Hamada-nakahara, S.; Suetsugu, S.
Deposited on : 2013-04-04
Resolution : 1.90 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 ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) 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

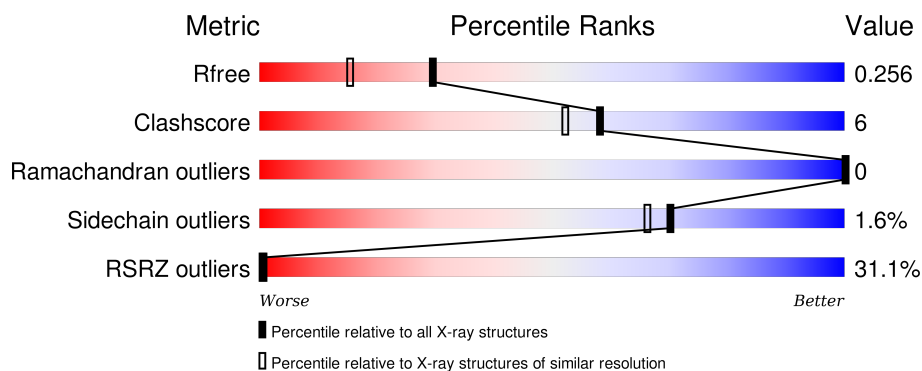
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	4755 (1.90-1.90)
Clashscore	102246	5398 (1.90-1.90)
Ramachandran outliers	100387	5338 (1.90-1.90)
Sidechain outliers	100360	5339 (1.90-1.90)
RSRZ outliers	91569	4766 (1.90-1.90)

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 $\leq 5\%$. 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	260	<div> <div>12%</div> <div>88%</div> <div>10%</div> <div>.</div> </div>
1	B	260	<div> <div>16%</div> <div>85%</div> <div>12%</div> <div>.</div> </div>
1	C	260	<div> <div>34%</div> <div>79%</div> <div>16%</div> <div>..</div> </div>
1	D	260	<div> <div>59%</div> <div>75%</div> <div>20%</div> <div>..</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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	I3P	D	2001	-	-	-	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8642 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 Vanilloid receptor-related osmotically activated channel protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	255	Total	C	N	O	S	0	8	0
			2058	1302	379	368	9			
1	B	255	Total	C	N	O	S	0	6	0
			2049	1296	376	368	9			
1	C	249	Total	C	N	O	S	0	1	0
			1989	1263	361	357	8			
1	D	249	Total	C	N	O	S	0	1	0
			1989	1261	365	355	8			

There are 40 discrepancies between the modelled and reference sequences:

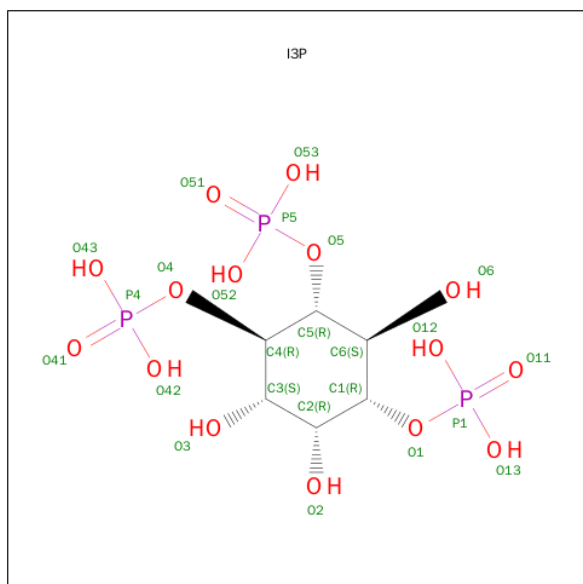
Chain	Residue	Modelled	Actual	Comment	Reference
A	132	MET	-	EXPRESSION TAG	UNP Q9DFS3
A	383	ALA	-	EXPRESSION TAG	UNP Q9DFS3
A	384	ALA	-	EXPRESSION TAG	UNP Q9DFS3
A	385	ALA	-	EXPRESSION TAG	UNP Q9DFS3
A	386	HIS	-	EXPRESSION TAG	UNP Q9DFS3
A	387	HIS	-	EXPRESSION TAG	UNP Q9DFS3
A	388	HIS	-	EXPRESSION TAG	UNP Q9DFS3
A	389	HIS	-	EXPRESSION TAG	UNP Q9DFS3
A	390	HIS	-	EXPRESSION TAG	UNP Q9DFS3
A	391	HIS	-	EXPRESSION TAG	UNP Q9DFS3
B	132	MET	-	EXPRESSION TAG	UNP Q9DFS3
B	383	ALA	-	EXPRESSION TAG	UNP Q9DFS3
B	384	ALA	-	EXPRESSION TAG	UNP Q9DFS3
B	385	ALA	-	EXPRESSION TAG	UNP Q9DFS3
B	386	HIS	-	EXPRESSION TAG	UNP Q9DFS3
B	387	HIS	-	EXPRESSION TAG	UNP Q9DFS3
B	388	HIS	-	EXPRESSION TAG	UNP Q9DFS3
B	389	HIS	-	EXPRESSION TAG	UNP Q9DFS3
B	390	HIS	-	EXPRESSION TAG	UNP Q9DFS3
B	391	HIS	-	EXPRESSION TAG	UNP Q9DFS3
C	132	MET	-	EXPRESSION TAG	UNP Q9DFS3

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Chain	Residue	Modelled	Actual	Comment	Reference
C	383	ALA	-	EXPRESSION TAG	UNP Q9DFS3
C	384	ALA	-	EXPRESSION TAG	UNP Q9DFS3
C	385	ALA	-	EXPRESSION TAG	UNP Q9DFS3
C	386	HIS	-	EXPRESSION TAG	UNP Q9DFS3
C	387	HIS	-	EXPRESSION TAG	UNP Q9DFS3
C	388	HIS	-	EXPRESSION TAG	UNP Q9DFS3
C	389	HIS	-	EXPRESSION TAG	UNP Q9DFS3
C	390	HIS	-	EXPRESSION TAG	UNP Q9DFS3
C	391	HIS	-	EXPRESSION TAG	UNP Q9DFS3
D	132	MET	-	EXPRESSION TAG	UNP Q9DFS3
D	383	ALA	-	EXPRESSION TAG	UNP Q9DFS3
D	384	ALA	-	EXPRESSION TAG	UNP Q9DFS3
D	385	ALA	-	EXPRESSION TAG	UNP Q9DFS3
D	386	HIS	-	EXPRESSION TAG	UNP Q9DFS3
D	387	HIS	-	EXPRESSION TAG	UNP Q9DFS3
D	388	HIS	-	EXPRESSION TAG	UNP Q9DFS3
D	389	HIS	-	EXPRESSION TAG	UNP Q9DFS3
D	390	HIS	-	EXPRESSION TAG	UNP Q9DFS3
D	391	HIS	-	EXPRESSION TAG	UNP Q9DFS3

- Molecule 2 is D-MYO-INOSITOL-1,4,5-TRIPHOSPHATE (three-letter code: I3P) (formula: $C_6H_{15}O_{15}P_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	P	0	0
			24	6	15	3		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	O	P	0	0
			24	6	15	3		
2	C	1	Total	C	O	P	0	0
			24	6	15	3		
2	D	1	Total	C	O	P	0	0
			24	6	15	3		

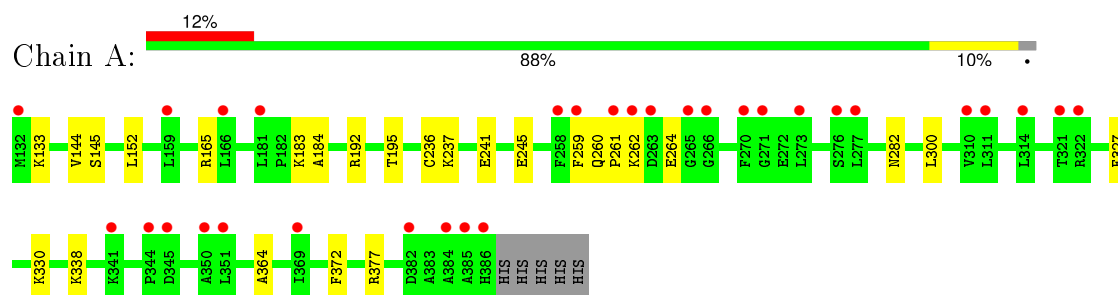
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	244	Total	O	0	0
			244	244		
3	B	201	Total	O	0	0
			201	201		
3	C	15	Total	O	0	0
			15	15		
3	D	1	Total	O	0	0
			1	1		

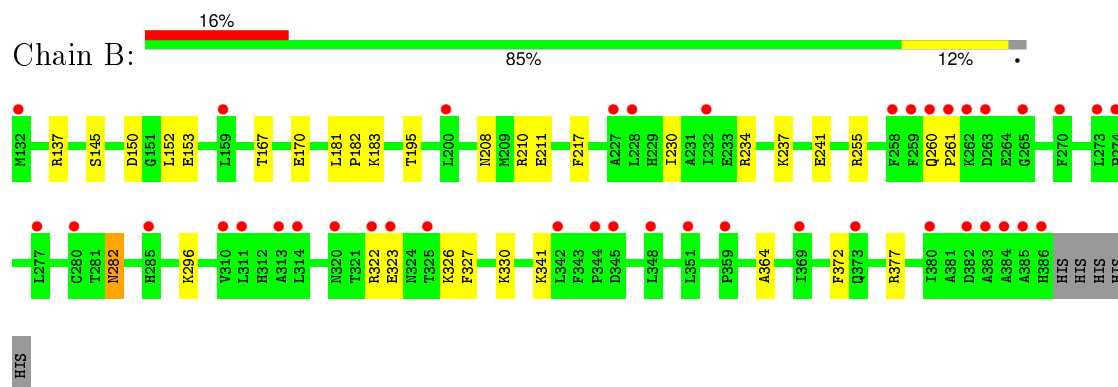
3 Residue-property plots

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

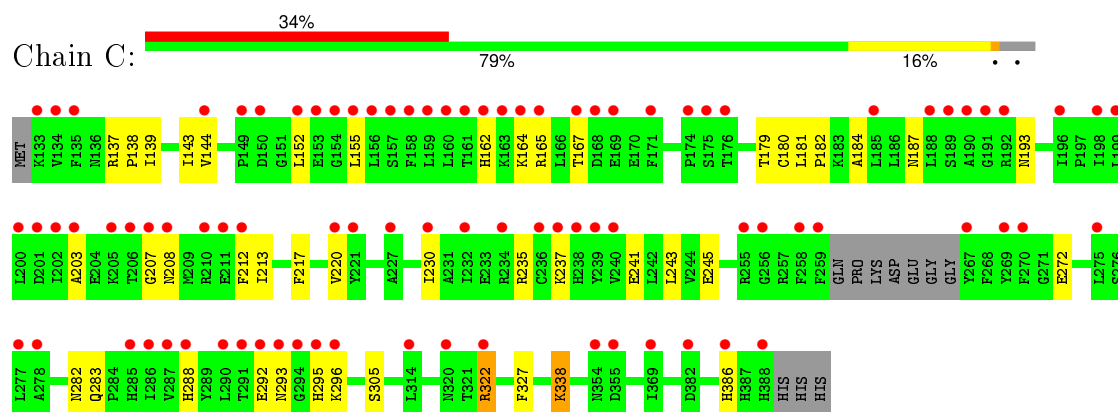
- Molecule 1: Vanilloid receptor-related osmotically activated channel protein



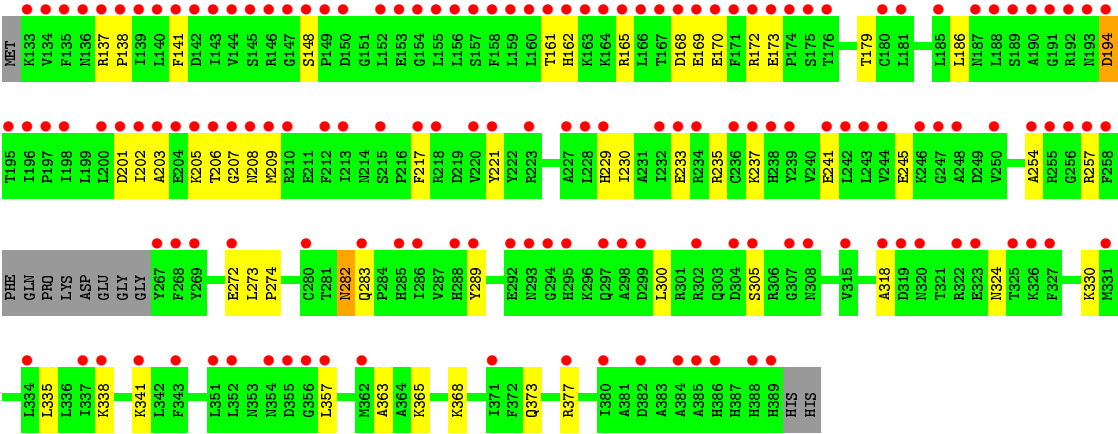
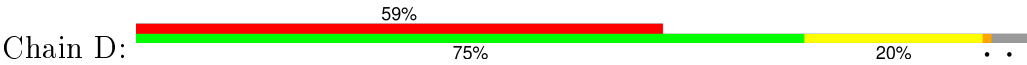
- Molecule 1: Vanilloid receptor-related osmotically activated channel protein



- Molecule 1: Vanilloid receptor-related osmotically activated channel protein



- Molecule 1: Vanilloid receptor-related osmotically activated channel protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	105.09Å 48.34Å 132.15Å 90.00° 101.44° 90.00°	Depositor
Resolution (Å)	32.81 – 1.90 32.81 – 1.90	Depositor EDS
% Data completeness (in resolution range)	96.7 (32.81-1.90) 92.8 (32.81-1.90)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.48 (at 1.89Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.218 , 0.246 0.228 , 0.256	Depositor DCC
R_{free} test set	2049 reflections (2.17%)	DCC
Wilson B-factor (Å ²)	25.2	Xtriage
Anisotropy	0.511	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 61.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 100699 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	8642	wwPDB-VP
Average B, all atoms (Å ²)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 67.06 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 5.4693e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: I3P

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	0.49	0/2139	0.63	0/2884
1	B	0.48	0/2120	0.65	0/2859
1	C	0.34	0/2034	0.58	0/2745
1	D	0.31	0/2035	0.60	0/2747
All	All	0.42	0/8328	0.62	0/11235

There are no bond length outliers.

There are no bond angle outliers.

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	2058	0	2096	17	0
1	B	2049	0	2080	21	0
1	C	1989	0	2008	24	0
1	D	1989	0	2007	37	0
2	A	24	0	9	1	0
2	B	24	0	9	2	0
2	C	24	0	9	0	0
2	D	24	0	9	3	0
3	A	244	0	0	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	201	0	0	5	0
3	C	15	0	0	0	0
3	D	1	0	0	0	0
All	All	8642	0	8227	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 6.

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:D:172:ARG:HG2	1:D:179:THR:HG22	1.66	0.77
1:A:192[A]:ARG:NH1	3:A:2214:HOH:O	2.24	0.69
1:C:292[B]:GLU:OE1	1:C:338:LYS:NZ	2.26	0.69
1:D:330:LYS:NZ	2:D:2001:I3P:O13	2.26	0.68
1:A:377:ARG:NH2	3:A:2319:HOH:O	2.26	0.68
1:B:322:ARG:NH1	1:B:323:GLU:OE1	2.29	0.66
1:D:203:ALA:O	1:D:208:ASN:N	2.28	0.66
1:B:210:ARG:NH1	3:B:2258:HOH:O	2.25	0.65
1:D:237:LYS:NZ	2:D:2001:I3P:O51	2.26	0.65
1:D:201:ASP:OD2	1:D:205:LYS:NZ	2.20	0.65
1:B:377:ARG:NH2	3:B:2284:HOH:O	2.30	0.65
1:A:237:LYS:NZ	3:A:2295:HOH:O	2.29	0.63
1:D:221:TYR:O	1:D:257:ARG:N	2.32	0.61
1:C:322:ARG:HD3	1:D:165:ARG:HD2	1.84	0.60
1:B:330:LYS:NZ	2:B:2001:I3P:O13	2.35	0.59
1:C:144:VAL:HG21	1:C:180:CYS:HB2	1.84	0.57
1:C:288:HIS:O	1:C:292[B]:GLU:HG2	2.03	0.57
1:D:165:ARG:NH2	1:D:207:GLY:O	2.37	0.57
1:C:217:PHE:CZ	1:C:230:ILE:HD11	2.40	0.57
1:D:300:LEU:HD21	1:D:335:LEU:HD22	1.87	0.56
1:C:208:ASN:ND2	1:C:212:PHE:HB2	2.21	0.55
1:D:272:GLU:OE2	1:D:305:SER:OG	2.18	0.55
1:D:194:ASP:N	1:D:194:ASP:OD2	2.31	0.54
1:A:165[A]:ARG:NH2	1:C:386:HIS:HB3	2.23	0.54
1:C:245:GLU:HG2	1:C:295:HIS:NE2	2.23	0.54
1:A:152:LEU:HD11	1:A:195:THR:HB	1.88	0.53
1:D:169:GLU:HA	1:D:172:ARG:HE	1.73	0.53
1:D:237:LYS:O	1:D:241:GLU:HG3	2.09	0.53
1:C:144:VAL:HG13	1:C:184:ALA:HB2	1.90	0.53
1:D:202:ILE:O	1:D:206:THR:N	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:237:LYS:O	1:C:241:GLU:HG3	2.10	0.52
1:A:300:LEU:HD11	1:A:338:LYS:HG2	1.92	0.51
1:D:229:HIS:ND1	1:D:254:ALA:HB2	2.26	0.51
1:D:318:ALA:HA	1:D:324:ASN:OD1	2.10	0.51
1:D:373:GLN:O	1:D:377:ARG:HG3	2.10	0.51
1:D:363:ALA:O	1:D:368:LYS:N	2.41	0.51
1:C:203:ALA:O	1:C:208:ASN:N	2.44	0.51
1:D:282:ASN:ND2	2:D:2001:I3P:O12	2.39	0.50
1:D:229:HIS:CD2	1:D:274:PRO:HG3	2.47	0.49
1:A:330:LYS:NZ	2:A:2001:I3P:O13	2.39	0.49
1:B:322:ARG:CZ	1:B:326:LYS:HD2	2.43	0.49
1:C:152:LEU:HD22	1:C:155:LEU:HD22	1.93	0.49
1:C:293:ASN:ND2	1:C:296:LYS:O	2.36	0.49
1:A:260:GLN:HB3	1:A:261:PRO:HD2	1.95	0.49
1:B:364:ALA:HB2	1:B:372:PHE:CE1	2.47	0.48
1:B:217:PHE:CZ	1:B:230:ILE:HD11	2.49	0.47
1:A:364:ALA:HB2	1:A:372:PHE:CE1	2.49	0.47
1:C:181:LEU:HD21	1:C:243:LEU:HD21	1.97	0.46
1:D:241:GLU:O	1:D:245:GLU:N	2.33	0.46
1:B:145:SER:HB3	1:B:183:LYS:HE3	1.98	0.46
1:C:235:ARG:NH2	1:C:283:GLN:HG2	2.30	0.46
1:B:211:GLU:N	1:B:211:GLU:OE1	2.37	0.46
1:C:213:ILE:HG23	1:C:243:LEU:HD22	1.98	0.45
1:D:137:ARG:HB3	1:D:138:PRO:HD3	1.98	0.45
1:B:260:GLN:HB3	1:B:261:PRO:HD2	1.97	0.45
1:D:229:HIS:CE1	1:D:254:ALA:HB2	2.51	0.45
1:D:141:PHE:HE2	1:D:173:GLU:HB2	1.83	0.44
1:B:341:LYS:NZ	3:B:2231:HOH:O	2.51	0.44
1:C:187:ASN:O	1:C:193:ASN:ND2	2.50	0.44
1:C:272:GLU:OE2	1:C:305:SER:OG	2.26	0.44
1:D:233:GLU:OE1	1:D:233:GLU:HA	2.18	0.44
1:C:139:ILE:O	1:C:143:ILE:HG13	2.18	0.43
1:D:141:PHE:CE2	1:D:173:GLU:HB2	2.53	0.43
1:D:203:ALA:HB1	1:D:209:MET:HA	2.00	0.43
1:C:165:ARG:NH2	1:C:207:GLY:O	2.44	0.43
1:C:179:THR:O	1:C:182:PRO:HD2	2.19	0.43
1:A:259:PHE:N	1:A:264:GLU:OE1	2.40	0.43
1:D:168:ASP:HB3	1:D:170:GLU:HG2	2.00	0.42
1:A:144:VAL:HG13	1:A:184:ALA:HB2	2.01	0.42
1:D:338:LYS:O	1:D:341:LYS:HB3	2.18	0.42
1:D:217:PHE:HZ	1:D:230:ILE:HD11	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:145:SER:HB3	1:A:183:LYS:HE3	2.02	0.42
1:D:235:ARG:NH2	1:D:283:GLN:HG2	2.34	0.42
1:B:296:LYS:HE2	1:B:296:LYS:HB2	1.81	0.42
1:A:133:LYS:HE2	3:A:2175:HOH:O	2.20	0.42
1:B:255:ARG:NH1	3:B:2138:HOH:O	2.32	0.41
1:A:262:LYS:HD3	1:A:262:LYS:HA	1.89	0.41
1:B:150:ASP:O	1:B:153:GLU:HG3	2.20	0.41
1:D:357:LEU:HD11	1:D:365:LYS:HD3	2.02	0.41
1:B:167:THR:HG23	1:B:208:ASN:HD21	1.85	0.41
1:C:162:HIS:HB3	1:C:164:LYS:NZ	2.35	0.41
1:A:237:LYS:O	1:A:241:GLU:HG3	2.20	0.41
1:B:282:ASN:ND2	2:B:2001:I3P:O12	2.53	0.41
1:D:186:LEU:HA	1:D:186:LEU:HD23	1.90	0.41
1:A:245:GLU:OE1	3:A:2185:HOH:O	2.22	0.41
1:B:237:LYS:O	1:B:241:GLU:HG3	2.20	0.41
1:D:137:ARG:HB2	1:D:170:GLU:O	2.21	0.41
1:B:181:LEU:HB3	1:B:182:PRO:HD3	2.03	0.41
1:C:144:VAL:HG11	1:C:180:CYS:O	2.20	0.41
1:D:241:GLU:HA	1:D:289:TYR:CE2	2.56	0.41
1:B:210:ARG:NH1	3:B:2265:HOH:O	2.46	0.40
1:D:273:LEU:HA	1:D:274:PRO:HD3	1.96	0.40
1:B:137:ARG:HB2	1:B:170:GLU:O	2.21	0.40
1:B:152:LEU:HD11	1:B:195:THR:HB	2.03	0.40
1:D:161:THR:HG22	1:D:162:HIS:ND1	2.37	0.40
1:A:236:CYS:HB3	3:A:2340:HOH:O	2.22	0.40
1:C:137:ARG:HB3	1:C:138:PRO:HD3	2.03	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	261/260 (100%)	255 (98%)	6 (2%)	0	100	100
1	B	259/260 (100%)	252 (97%)	7 (3%)	0	100	100
1	C	246/260 (95%)	238 (97%)	8 (3%)	0	100	100
1	D	246/260 (95%)	238 (97%)	8 (3%)	0	100	100
All	All	1012/1040 (97%)	983 (97%)	29 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	224/221 (101%)	222 (99%)	2 (1%)	84	83
1	B	222/221 (100%)	218 (98%)	4 (2%)	66	61
1	C	213/221 (96%)	207 (97%)	6 (3%)	51	41
1	D	213/221 (96%)	210 (99%)	3 (1%)	74	71
All	All	872/884 (99%)	857 (98%)	15 (2%)	70	64

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	282	ASN
1	A	327	PHE
1	B	234[A]	ARG
1	B	234[B]	ARG
1	B	282	ASN
1	B	327	PHE
1	C	167	THR
1	C	220	VAL
1	C	282	ASN
1	C	322	ARG
1	C	327	PHE
1	C	338	LYS
1	D	148	SER

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Mol	Chain	Res	Type
1	D	194	ASP
1	D	282	ASN

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

Mol	Chain	Res	Type
1	B	208	ASN
1	C	282	ASN
1	C	285	HIS

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](#)

4 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	I3P	A	2001	-	24,24,24	0.96	0	33,39,39	0.78	0
2	I3P	B	2001	-	24,24,24	0.89	0	33,39,39	0.82	1 (3%)
2	I3P	C	2001	-	24,24,24	0.93	0	33,39,39	1.00	0
2	I3P	D	2001	-	24,24,24	0.90	0	33,39,39	0.95	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
2	I3P	A	2001	-	-	0/15/39/39	0/1/1/1
2	I3P	B	2001	-	-	0/15/39/39	0/1/1/1
2	I3P	C	2001	-	-	0/15/39/39	0/1/1/1
2	I3P	D	2001	-	-	0/15/39/39	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2001	I3P	C2-C3-C4	2.17	114.36	109.60

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	2001	I3P	1	0
2	B	2001	I3P	2	0
2	D	2001	I3P	3	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, 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	255/260 (98%)	0.69	31 (12%) 5 6	17, 29, 62, 98	0
1	B	255/260 (98%)	0.96	41 (16%) 3 3	19, 35, 84, 131	0
1	C	249/260 (95%)	1.77	88 (35%) 0 0	38, 78, 113, 161	0
1	D	249/260 (95%)	3.08	153 (61%) 0 0	62, 106, 140, 157	0
All	All	1008/1040 (96%)	1.61	313 (31%) 1 0	17, 61, 129, 161	0

All (313) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	139	ILE	14.1
1	D	157	SER	13.2
1	C	258	PHE	12.0
1	D	159	LEU	9.6
1	B	386	HIS	9.4
1	D	166	LEU	8.9
1	D	160	LEU	8.7
1	D	323	GLU	8.7
1	D	285	HIS	8.7
1	D	198	ILE	8.6
1	B	384	ALA	8.5
1	D	156	LEU	8.3
1	C	388	HIS	8.3
1	D	152	LEU	7.9
1	D	389	HIS	7.6
1	D	133	LYS	7.5
1	D	134	VAL	7.4
1	C	158	PHE	7.4
1	D	170	GLU	7.3
1	D	238	HIS	7.3
1	C	207	GLY	7.3

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Mol	Chain	Res	Type	RSRZ
1	D	161	THR	7.3
1	D	289	TYR	7.3
1	C	190	ALA	7.2
1	B	383	ALA	7.1
1	D	195	THR	7.1
1	D	171	PHE	7.0
1	B	132	MET	6.7
1	C	162	HIS	6.7
1	D	207	GLY	6.6
1	D	162	HIS	6.6
1	A	262	LYS	6.5
1	D	205	LYS	6.4
1	D	294	GLY	6.4
1	D	155	LEU	6.4
1	D	176	THR	6.3
1	C	259	PHE	6.2
1	C	134	VAL	6.2
1	A	385	ALA	6.2
1	D	167	THR	6.2
1	D	232	ILE	6.2
1	C	208	ASN	6.1
1	C	152	LEU	6.0
1	C	161	THR	5.9
1	D	388	HIS	5.9
1	D	189	SER	5.8
1	D	175	SER	5.8
1	D	172	ARG	5.7
1	C	163	LYS	5.7
1	D	295	HIS	5.6
1	C	155	LEU	5.5
1	D	292	GLU	5.5
1	D	286	ILE	5.5
1	D	298	ALA	5.5
1	D	190	ALA	5.4
1	D	192	ARG	5.4
1	A	386	HIS	5.4
1	B	261	PRO	5.3
1	C	196	ILE	5.2
1	A	261	PRO	5.2
1	C	192	ARG	5.1
1	B	322	ARG	4.9
1	D	385	ALA	4.9

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Mol	Chain	Res	Type	RSRZ
1	D	213	ILE	4.9
1	D	158	PHE	4.9
1	D	164	LYS	4.8
1	D	191	GLY	4.8
1	D	193	ASN	4.8
1	D	153	GLU	4.8
1	D	144	VAL	4.8
1	D	150	ASP	4.8
1	D	188	LEU	4.8
1	C	160	LEU	4.8
1	D	196	ILE	4.8
1	D	201	ASP	4.7
1	D	221	TYR	4.7
1	D	149	PRO	4.7
1	C	159	LEU	4.7
1	D	305	SER	4.7
1	C	295	HIS	4.7
1	B	262	LYS	4.7
1	D	197	PRO	4.6
1	C	202	ILE	4.6
1	D	237	LYS	4.5
1	D	307	GLY	4.5
1	D	210	ARG	4.5
1	C	369	ILE	4.5
1	D	257	ARG	4.4
1	D	386	HIS	4.4
1	D	141	PHE	4.4
1	D	200	LEU	4.3
1	D	135	PHE	4.3
1	C	320	ASN	4.3
1	D	154	GLY	4.3
1	D	163	LYS	4.3
1	C	149	PRO	4.3
1	B	345	ASP	4.3
1	C	157	SER	4.2
1	D	212	PHE	4.2
1	C	188	LEU	4.2
1	D	256	GLY	4.2
1	D	239	TYR	4.2
1	C	164	LYS	4.1
1	D	185	LEU	4.1
1	D	357	LEU	4.1

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Mol	Chain	Res	Type	RSRZ
1	B	258	PHE	4.1
1	C	165	ARG	4.0
1	D	337	ILE	4.0
1	B	385	ALA	4.0
1	D	181	LEU	3.9
1	C	167	THR	3.9
1	D	355	ASP	3.9
1	A	258	PHE	3.9
1	D	220	VAL	3.8
1	D	293	ASN	3.8
1	D	255	ARG	3.8
1	D	384	ALA	3.8
1	A	310	VAL	3.8
1	C	236	CYS	3.8
1	D	247	GLY	3.8
1	D	174	PRO	3.8
1	D	283	GLN	3.7
1	C	355	ASP	3.7
1	D	140	LEU	3.7
1	D	209	MET	3.7
1	D	187	ASN	3.7
1	C	210	ARG	3.6
1	D	169	GLU	3.6
1	D	142	ASP	3.6
1	D	338	LYS	3.6
1	C	221	TYR	3.6
1	C	294	GLY	3.6
1	D	297	GLN	3.6
1	C	205	LYS	3.6
1	D	223	ARG	3.6
1	A	266	GLY	3.6
1	D	136	ASN	3.6
1	D	267	TYR	3.5
1	D	351	LEU	3.5
1	B	310	VAL	3.5
1	A	384	ALA	3.5
1	C	354	ASN	3.5
1	A	345	ASP	3.4
1	C	256	GLY	3.4
1	B	382	ASP	3.3
1	C	156	LEU	3.3
1	D	148	SER	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	380	ILE	3.3
1	C	296	LYS	3.3
1	D	356	GLY	3.3
1	D	217	PHE	3.3
1	B	313	ALA	3.3
1	D	322	ARG	3.3
1	D	382	ASP	3.2
1	D	258	PHE	3.2
1	D	246	LYS	3.2
1	D	208	ASN	3.2
1	B	263	ASP	3.2
1	D	354	ASN	3.2
1	C	176	THR	3.2
1	D	341	LYS	3.2
1	A	265	GLY	3.2
1	C	171	PHE	3.2
1	A	344	PRO	3.2
1	B	320	ASN	3.2
1	C	234	ARG	3.1
1	D	254	ALA	3.1
1	C	240	VAL	3.1
1	B	351	LEU	3.1
1	B	270	PHE	3.1
1	D	343	PHE	3.1
1	C	239	TYR	3.1
1	C	201	ASP	3.1
1	C	322	ARG	3.1
1	C	199	LEU	3.1
1	D	352	LEU	3.1
1	C	285	HIS	3.1
1	D	194	ASP	3.1
1	B	273	LEU	3.1
1	C	291	THR	3.1
1	B	260	GLN	3.1
1	C	191	GLY	3.1
1	A	311	LEU	3.0
1	C	198	ILE	3.0
1	B	373	GLN	3.0
1	D	165	ARG	3.0
1	D	371	ILE	3.0
1	C	267	TYR	3.0
1	D	168	ASP	3.0

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Mol	Chain	Res	Type	RSRZ
1	C	133	LYS	3.0
1	D	147	GLY	3.0
1	C	144	VAL	3.0
1	D	308	ASN	3.0
1	C	169	GLU	2.9
1	A	273	LEU	2.9
1	C	206	THR	2.9
1	D	280	CYS	2.9
1	D	233	GLU	2.9
1	D	334	LEU	2.9
1	D	327	PHE	2.8
1	D	143	ILE	2.8
1	D	206	THR	2.8
1	D	315	VAL	2.8
1	B	259	PHE	2.8
1	C	275	LEU	2.8
1	D	325	THR	2.8
1	B	277	LEU	2.7
1	D	138	PRO	2.7
1	D	318	ALA	2.7
1	C	200	LEU	2.7
1	D	248	ALA	2.7
1	C	277	LEU	2.7
1	D	146	ARG	2.7
1	C	150	ASP	2.7
1	D	319	ASP	2.7
1	D	244	VAL	2.7
1	C	269	TYR	2.7
1	B	325	THR	2.6
1	D	236	CYS	2.6
1	D	269	TYR	2.6
1	C	278	ALA	2.6
1	C	212	PHE	2.6
1	B	285	HIS	2.6
1	C	255	ARG	2.6
1	D	302	ARG	2.6
1	B	311	LEU	2.6
1	D	204	GLU	2.6
1	C	238	HIS	2.6
1	C	227	ALA	2.5
1	D	234	ARG	2.5
1	D	243	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	227	ALA	2.5
1	D	215	SER	2.5
1	C	230	ILE	2.5
1	B	265	GLY	2.5
1	C	237	LYS	2.5
1	D	241	GLU	2.5
1	C	287	VAL	2.5
1	D	218	ARG	2.5
1	B	314	LEU	2.5
1	D	228	LEU	2.5
1	A	132	MET	2.5
1	D	137	ARG	2.5
1	A	369	ILE	2.4
1	B	359	PRO	2.4
1	C	135	PHE	2.4
1	D	320	ASN	2.4
1	B	342	LEU	2.4
1	D	242	LEU	2.4
1	C	211	GLU	2.4
1	D	180	CYS	2.4
1	D	304	ASP	2.4
1	A	350	ALA	2.4
1	B	227	ALA	2.4
1	D	202	ILE	2.4
1	A	159	LEU	2.4
1	A	351	LEU	2.4
1	D	326	LYS	2.4
1	C	220	VAL	2.4
1	D	145	SER	2.4
1	C	314	LEU	2.3
1	B	232	ILE	2.3
1	D	362	MET	2.3
1	C	286	ILE	2.3
1	C	189	SER	2.3
1	D	272	GLU	2.3
1	C	293	ASN	2.3
1	A	259	PHE	2.3
1	A	263	ASP	2.3
1	B	200	LEU	2.2
1	B	280	CYS	2.2
1	C	382	ASP	2.2
1	D	288	HIS	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	153	GLU	2.2
1	D	173	GLU	2.2
1	B	228	LEU	2.2
1	C	185	LEU	2.2
1	B	274	PRO	2.2
1	D	380	ILE	2.2
1	A	277[A]	LEU	2.2
1	D	331	MET	2.2
1	A	276	SER	2.2
1	C	175	SER	2.2
1	A	270	PHE	2.2
1	C	154	GLY	2.2
1	C	270	PHE	2.2
1	A	382	ASP	2.2
1	C	232	ILE	2.1
1	A	314	LEU	2.1
1	C	168	ASP	2.1
1	B	369	ILE	2.1
1	B	159	LEU	2.1
1	B	348	LEU	2.1
1	D	203	ALA	2.1
1	A	321	THR	2.1
1	D	377	ARG	2.1
1	A	181	LEU	2.1
1	D	299	ASP	2.1
1	C	174	PRO	2.1
1	A	166	LEU	2.1
1	C	290	LEU	2.1
1	A	341	LYS	2.1
1	B	323	GLU	2.1
1	A	271	GLY	2.1
1	D	268	PHE	2.0
1	C	203	ALA	2.0
1	C	386	HIS	2.0
1	B	344	PRO	2.0
1	C	292[A]	GLU	2.0
1	C	288	HIS	2.0
1	A	322	ARG	2.0
1	D	250	VAL	2.0
1	D	229	HIS	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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	LLDF	B-factors(\AA^2)	Q<0.9
2	I3P	A	2001	24/24	0.88	0.20	1.95	51,66,73,77	0
2	I3P	B	2001	24/24	0.73	0.27	1.68	79,86,108,110	0
2	I3P	D	2001	24/24	0.65	0.43	0.87	87,95,120,121	0
2	I3P	C	2001	24/24	0.86	0.23	0.59	68,79,94,96	0

6.5 Other polymers [i](#)

There are no such residues in this entry.