Full wwPDB X-ray Structure Validation Report

Feb 1, 2016 – 04:39 AM GMT

PDB ID	:	2NQ2
Title	:	An inward-facing conformation of a putative metal-chelate type ABC transporter.
Authors	:	Pinkett, H.P.; Lee, A.T.; Lum, P.; Locher, K.P.; Rees, D.C.
Deposited on	:	2006-10-30
Resolution	:	2.40 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

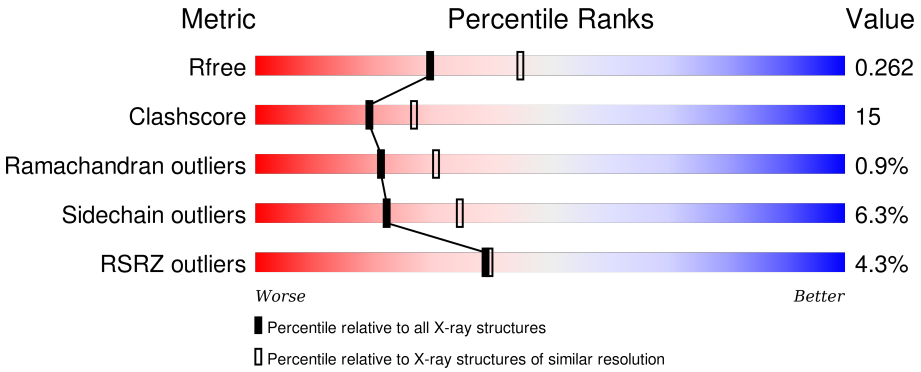
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	2919 (2.40-2.40)
Clashscore	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)
RSRZ outliers	91569	2928 (2.40-2.40)

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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	337	4% 58% 29% • 9%
1	B	337	4% 61% 26% • 11%
2	C	253	4% 74% 21% • •
2	D	253	4% 74% 21% • •

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9249 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 Hypothetical ABC transporter permease protein HI1471.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	308	Total	C	N	O	S	34	0	0
			2347	1575	366	395	11			
1	B	300	Total	C	N	O	S	34	0	0
			2258	1513	353	381	11			

- Molecule 2 is a protein called Hypothetical ABC transporter ATP-binding protein HI1470.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	251	Total	C	N	O	S	23	0	0
			1995	1291	332	366	6			
2	D	248	Total	C	N	O	S	16	0	0
			1967	1272	328	360	7			

- Molecule 3 is water.

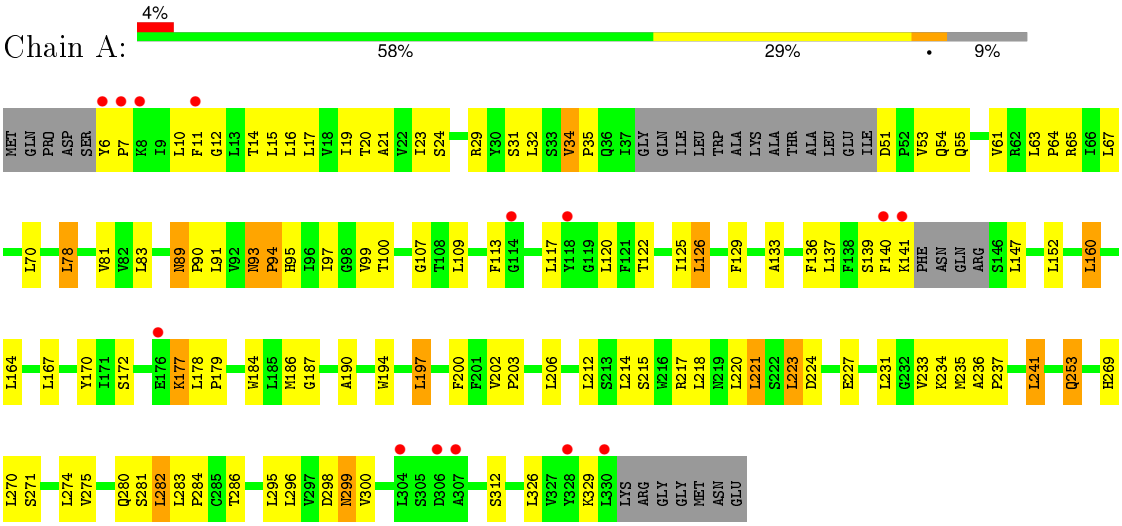
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	142	Total	O	0	0
			142	142		
3	B	162	Total	O	0	0
			162	162		
3	C	170	Total	O	0	0
			170	170		
3	D	208	Total	O	0	0
			208	208		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

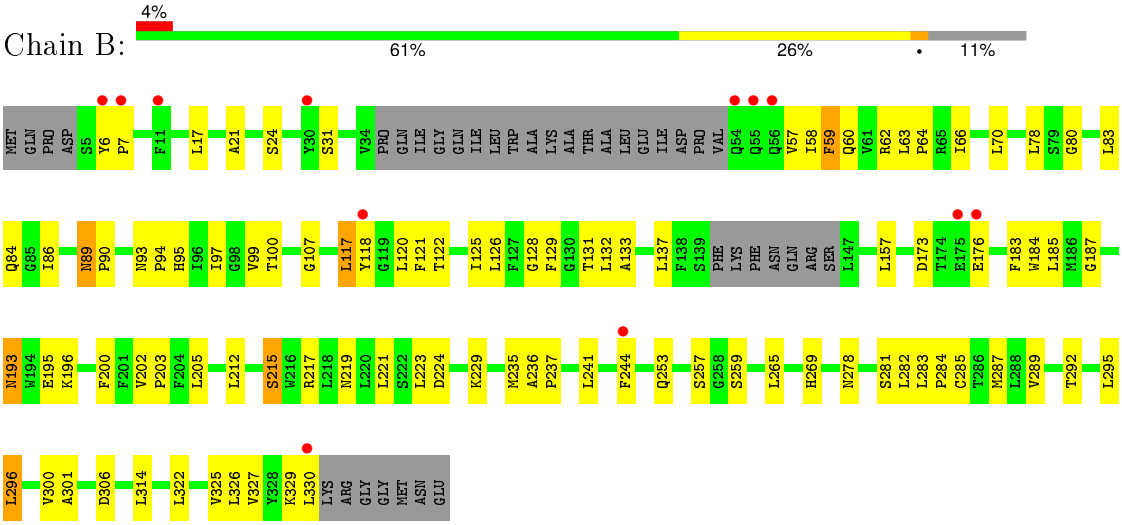
• Molecule 1: Hypothetical ABC transporter permease protein HI1471

Chain A:



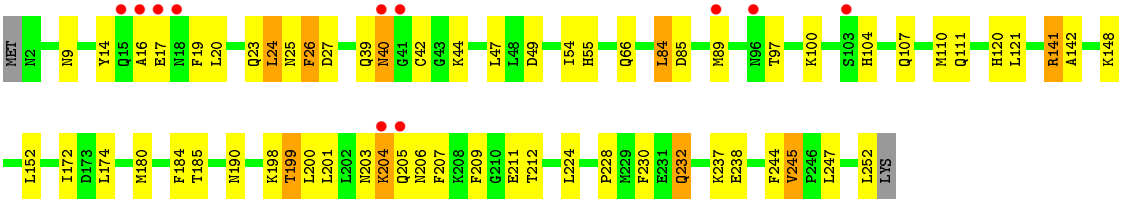
• Molecule 1: Hypothetical ABC transporter permease protein HI1471

Chain B:



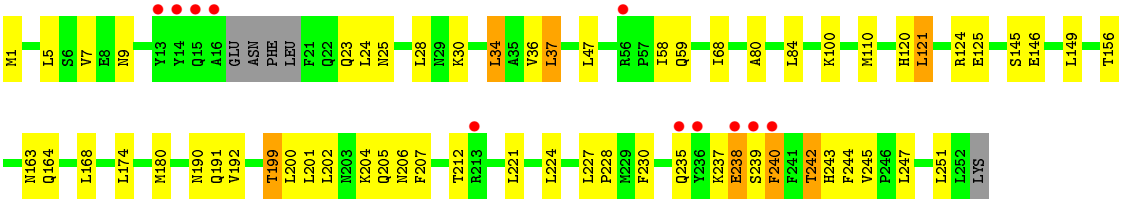
• Molecule 2: Hypothetical ABC transporter ATP-binding protein HI1470

Chain C:



- Molecule 2: Hypothetical ABC transporter ATP-binding protein HI1470

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	97.85Å 142.47Å 150.27Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	28.00 – 2.40 27.99 – 2.40	Depositor EDS
% Data completeness (in resolution range)	98.9 (28.00-2.40) 99.0 (27.99-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$< I/\sigma(I) >$ [1]	11.51 (at 2.39Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.222 , 0.260 0.225 , 0.262	Depositor DCC
R_{free} test set	8214 reflections (10.04%)	DCC
Wilson B-factor (Å^2)	43.3	Xtriage
Anisotropy	0.286	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 61.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 81824 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	9249	wwPDB-VP
Average B, all atoms (Å^2)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.85% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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	0.33	0/2398	0.54	0/3262
1	B	0.33	0/2305	0.56	0/3136
2	C	0.38	0/2035	0.59	0/2758
2	D	0.41	0/2005	0.61	0/2715
All	All	0.36	0/8743	0.58	0/11871

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

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	2347	0	2506	94	0
1	B	2258	0	2397	77	0
2	C	1995	0	2020	48	0
2	D	1967	0	1999	47	0
3	A	142	0	0	0	0
3	B	162	0	0	1	0
3	C	170	0	0	0	0
3	D	208	0	0	2	0
All	All	9249	0	8922	258	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 15.

All (258) 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:51:ASP:N	1:A:55:GLN:H	1.58	0.99
1:B:212:LEU:HD11	1:B:287:MET:HE1	1.49	0.95
1:B:95:HIS:ND1	1:B:100:THR:HG21	1.90	0.86
2:D:9:ASN:HD22	2:D:23:GLN:HA	1.40	0.85
2:C:190:ASN:HD21	2:C:244:PHE:H	1.21	0.84
1:B:236:ALA:HB3	1:B:237:PRO:HD3	1.58	0.84
2:C:174:LEU:HD22	2:C:180:MET:CE	2.08	0.83
1:A:215:SER:HB3	2:C:100:LYS:HE3	1.61	0.82
1:B:89:ASN:HD22	1:B:90:PRO:HD2	1.49	0.76
1:A:95:HIS:CD2	1:A:100:THR:HG21	2.20	0.76
1:A:172:SER:HB2	1:A:177:LYS:HG2	1.67	0.76
1:A:282:LEU:O	1:A:286:THR:HG23	1.85	0.76
1:B:301:ALA:HB2	1:B:314:LEU:HD12	1.69	0.74
1:A:236:ALA:HB3	1:A:237:PRO:HD3	1.67	0.74
2:D:9:ASN:H	2:D:25:ASN:ND2	1.85	0.74
1:B:93:ASN:HB2	1:B:94:PRO:HD2	1.71	0.73
2:D:9:ASN:ND2	2:D:23:GLN:HA	2.04	0.73
1:B:219:ASN:HD21	1:B:278:ASN:ND2	1.87	0.73
1:A:212:LEU:O	1:A:215:SER:HB2	1.89	0.72
1:A:89:ASN:HD22	1:A:90:PRO:HD2	1.55	0.72
2:C:174:LEU:HD22	2:C:180:MET:HE1	1.70	0.72
2:D:68:ILE:HG12	2:D:149:LEU:HD23	1.72	0.71
1:A:221:LEU:HD12	1:A:235:MET:CE	2.20	0.71
1:B:21:ALA:O	1:B:24:SER:HB3	1.90	0.71
1:A:200:PHE:O	1:A:203:PRO:HD2	1.90	0.71
2:C:174:LEU:HD22	2:C:180:MET:HE3	1.73	0.71
2:D:9:ASN:HD21	2:D:23:GLN:HE21	1.39	0.71
1:B:193:ASN:ND2	1:B:196:LYS:H	1.89	0.70
2:C:44:LYS:HD3	2:C:185:THR:HB	1.74	0.70
1:A:215:SER:OG	1:A:280:GLN:HA	1.92	0.70
1:A:34:VAL:H	1:A:35:PRO:CD	2.04	0.70
1:B:89:ASN:HD22	1:B:90:PRO:CD	2.04	0.70
1:B:202:VAL:HB	1:B:203:PRO:HD3	1.75	0.69
1:A:299:ASN:C	1:A:299:ASN:HD22	1.94	0.69
1:B:62:ARG:HH21	1:B:62:ARG:HG3	1.58	0.68
1:B:6:TYR:HB3	1:B:7:PRO:HD3	1.75	0.68
2:C:42:CYS:SG	2:C:44:LYS:HG3	2.35	0.67
1:A:178:LEU:HB3	1:A:179:PRO:HD3	1.77	0.67
1:A:34:VAL:H	1:A:35:PRO:HD3	1.60	0.67
1:A:269:HIS:HD2	1:A:326:LEU:HD13	1.59	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:228:PRO:HG2	2:C:247:LEU:HB3	1.76	0.66
1:A:93:ASN:HB2	1:A:94:PRO:HD2	1.77	0.66
1:A:89:ASN:HD22	1:A:90:PRO:CD	2.09	0.66
1:B:322:LEU:O	1:B:325:VAL:HG22	1.96	0.66
2:D:36:VAL:HG13	2:D:200:LEU:HD12	1.78	0.65
2:D:200:LEU:CD1	2:D:202:LEU:HG	2.26	0.65
1:A:64:PRO:HG3	1:A:194:TRP:CE2	2.33	0.64
1:A:64:PRO:HG3	1:A:194:TRP:NE1	2.12	0.64
1:A:202:VAL:HB	1:A:203:PRO:HD3	1.79	0.64
1:B:118:TYR:O	1:B:122:THR:HG22	1.96	0.64
1:A:29:ARG:HG2	1:A:29:ARG:HH21	1.63	0.64
1:B:83:LEU:HD12	1:B:94:PRO:HA	1.79	0.63
2:C:190:ASN:ND2	2:C:244:PHE:H	1.96	0.63
2:D:120:HIS:CD2	2:D:121:LEU:HD13	2.34	0.63
2:D:230:PHE:HB3	2:D:245:VAL:HG13	1.80	0.62
1:A:271:SER:CB	1:A:286:THR:HG22	2.29	0.62
2:D:174:LEU:HD22	2:D:180:MET:CE	2.30	0.62
2:D:227:LEU:HD12	2:D:228:PRO:HD2	1.81	0.61
1:B:97:ILE:HG23	1:B:99:VAL:HG23	1.82	0.61
1:A:61:VAL:O	1:A:64:PRO:HD2	2.01	0.61
1:B:200:PHE:O	1:B:203:PRO:HD2	2.01	0.61
1:B:6:TYR:CE1	1:B:281:SER:HB2	2.36	0.60
2:D:237:LYS:O	2:D:238:GLU:HG3	2.02	0.60
2:C:14:TYR:CZ	2:C:16:ALA:HB3	2.36	0.60
1:A:89:ASN:ND2	1:A:91:LEU:H	2.00	0.59
1:A:34:VAL:N	1:A:35:PRO:CD	2.65	0.59
1:B:63:LEU:N	1:B:64:PRO:HD2	2.17	0.59
2:D:58:ILE:HG22	2:D:59:GLN:HG3	1.83	0.59
2:C:199:THR:HG23	2:C:212:THR:HA	1.85	0.58
1:B:212:LEU:HD21	1:B:287:MET:HE2	1.85	0.58
1:B:193:ASN:ND2	1:B:195:GLU:HB3	2.18	0.58
1:A:270:LEU:O	1:A:274:LEU:HD13	2.02	0.58
1:B:133:ALA:O	1:B:137:LEU:HD23	2.04	0.58
2:D:84:LEU:HD13	2:D:110:MET:HE3	1.86	0.58
2:C:14:TYR:CE2	2:C:16:ALA:HB3	2.39	0.57
1:A:296:LEU:O	1:A:300:VAL:HG23	2.04	0.57
1:B:219:ASN:HD21	1:B:278:ASN:HD22	1.52	0.57
1:A:63:LEU:HB3	1:A:64:PRO:HD3	1.87	0.57
1:A:78:LEU:O	1:A:81:VAL:HG12	2.05	0.57
1:A:83:LEU:CD1	1:A:94:PRO:HA	2.35	0.56
1:A:65:ARG:HD3	1:A:298:ASP:OD1	2.04	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:84:LEU:HD13	2:D:110:MET:CE	2.35	0.56
1:B:80:GLY:O	1:B:84:GLN:HG3	2.05	0.56
2:D:37:LEU:HG	2:D:192:VAL:HG21	1.87	0.56
1:A:122:THR:O	1:A:126:LEU:HB2	2.05	0.56
2:C:14:TYR:HE2	2:C:17:GLU:HG2	1.71	0.56
2:D:156:THR:HB	2:D:164:GLN:HG2	1.86	0.56
2:C:9:ASN:ND2	2:C:23:GLN:HG2	2.20	0.56
2:C:237:LYS:O	2:C:238:GLU:HB2	2.06	0.55
1:B:193:ASN:HD21	1:B:195:GLU:HB3	1.72	0.55
2:C:107:GLN:O	2:C:111:GLN:HG2	2.06	0.55
2:D:9:ASN:HD21	2:D:23:GLN:NE2	2.05	0.55
1:A:152:LEU:HD23	1:B:327:VAL:HG11	1.88	0.55
1:B:193:ASN:HD21	1:B:196:LYS:H	1.53	0.55
2:C:84:LEU:HG	2:C:110:MET:CE	2.37	0.54
2:C:230:PHE:CE1	2:C:245:VAL:HG22	2.43	0.54
1:A:51:ASP:N	1:A:55:GLN:N	2.42	0.54
1:B:107:GLY:HA3	1:B:184:TRP:CH2	2.42	0.54
1:B:212:LEU:O	1:B:215:SER:HB2	2.08	0.54
1:A:221:LEU:HD12	1:A:235:MET:HE1	1.89	0.54
2:C:247:LEU:HD11	2:C:252:LEU:HD11	1.89	0.54
1:B:129:PHE:HA	1:B:132:LEU:HD23	1.90	0.54
2:C:198:LYS:HE2	2:C:211:GLU:OE2	2.08	0.54
2:C:9:ASN:HD21	2:C:23:GLN:HG2	1.72	0.54
1:B:193:ASN:HD22	1:B:193:ASN:C	2.11	0.53
1:A:17:LEU:HD21	1:A:70:LEU:HD22	1.90	0.53
1:A:186:MET:O	1:A:312:SER:HB3	2.09	0.53
2:C:203:ASN:HB2	2:C:224:LEU:HD13	1.91	0.52
1:A:170:TYR:HA	1:B:183:PHE:CE1	2.45	0.52
2:C:199:THR:HG22	2:C:212:THR:OG1	2.10	0.52
1:B:131:THR:HG23	1:B:157:LEU:HD23	1.91	0.52
2:C:54:ILE:HG13	2:C:55:HIS:N	2.25	0.52
1:A:53:VAL:HG13	1:A:54:GLN:N	2.24	0.52
1:B:89:ASN:HD22	1:B:90:PRO:N	2.06	0.52
1:A:282:LEU:HD22	1:A:286:THR:CG2	2.40	0.52
2:D:9:ASN:H	2:D:25:ASN:HD21	1.57	0.51
1:A:93:ASN:HD22	1:A:93:ASN:C	2.13	0.51
2:C:66:GLN:HB3	2:C:148:LYS:HB2	1.93	0.51
2:D:200:LEU:HD11	2:D:202:LEU:HG	1.92	0.51
1:A:125:ILE:HG23	1:A:129:PHE:CE1	2.45	0.51
1:A:109:LEU:HD11	1:A:113:PHE:HE1	1.74	0.51
1:A:220:LEU:HD13	1:A:233:VAL:HG22	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:16:LEU:O	1:A:20:THR:HG23	2.10	0.51
1:B:187:GLY:HA2	1:B:257:SER:O	2.11	0.51
1:A:83:LEU:HD12	1:A:94:PRO:HA	1.92	0.51
1:B:6:TYR:OH	1:B:284:PRO:HG2	2.11	0.51
2:C:247:LEU:HD11	2:C:252:LEU:CD1	2.41	0.51
2:C:25:ASN:O	2:C:26:PHE:HB3	2.11	0.51
1:B:86:ILE:HG12	1:B:221:LEU:HD13	1.92	0.51
1:A:223:LEU:HD21	1:A:231:LEU:HD12	1.91	0.51
1:A:67:LEU:HB2	1:A:197:LEU:HD11	1.92	0.51
1:A:61:VAL:C	1:A:64:PRO:HD2	2.32	0.51
2:D:174:LEU:HD22	2:D:180:MET:HE1	1.93	0.51
1:B:83:LEU:CD1	1:B:94:PRO:HA	2.41	0.50
2:D:240:PHE:N	2:D:240:PHE:CD1	2.80	0.50
2:C:204:LYS:C	2:C:206:ASN:H	2.15	0.50
1:A:136:PHE:O	1:A:139:SER:HB3	2.10	0.50
1:A:11:PHE:HA	1:A:14:THR:HG22	1.94	0.50
1:A:19:ILE:O	1:A:23:ILE:HG13	2.11	0.50
2:D:5:LEU:HD12	2:D:5:LEU:C	2.32	0.50
1:B:70:LEU:HD21	1:B:295:LEU:HD22	1.92	0.49
1:A:275:VAL:O	1:A:275:VAL:HG22	2.12	0.49
1:A:31:SER:C	1:A:32:LEU:HD12	2.33	0.49
1:A:107:GLY:HA3	1:A:184:TRP:CH2	2.47	0.49
2:D:174:LEU:HD22	2:D:180:MET:HE3	1.93	0.49
2:C:141:ARG:HG3	2:C:142:ALA:N	2.28	0.49
1:A:275:VAL:HG21	1:A:281:SER:HB3	1.95	0.49
1:A:133:ALA:O	1:A:137:LEU:HD13	2.13	0.49
1:A:120:LEU:HD23	1:A:120:LEU:C	2.33	0.49
1:A:221:LEU:HD12	1:A:235:MET:HE2	1.93	0.49
1:A:89:ASN:HD22	1:A:90:PRO:N	2.10	0.48
1:A:65:ARG:NH2	1:A:190:ALA:HA	2.27	0.48
1:A:6:TYR:CZ	1:A:10:LEU:HD11	2.48	0.48
1:A:29:ARG:NH2	1:A:29:ARG:HG2	2.27	0.48
1:A:6:TYR:N	1:A:7:PRO:HD2	2.29	0.48
1:B:185:LEU:O	1:B:259:SER:HB3	2.13	0.48
1:B:215:SER:CB	2:D:100:LYS:HE3	2.44	0.48
1:A:271:SER:HB2	1:A:286:THR:HG22	1.94	0.48
1:B:327:VAL:C	1:B:329:LYS:H	2.15	0.48
1:B:89:ASN:ND2	1:B:90:PRO:HD2	2.26	0.47
1:B:301:ALA:HB2	1:B:314:LEU:CD1	2.42	0.47
2:C:24:LEU:HA	2:C:207:PHE:CZ	2.48	0.47
1:B:58:ILE:C	1:B:60:GLN:H	2.16	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:9:ASN:ND2	2:D:23:GLN:HG3	2.29	0.47
2:C:84:LEU:HG	2:C:110:MET:HE3	1.97	0.47
2:C:204:LYS:O	2:C:206:ASN:N	2.47	0.47
2:D:168:LEU:HD11	2:D:191:GLN:HG2	1.96	0.47
1:A:93:ASN:C	1:A:93:ASN:ND2	2.67	0.47
1:A:186:MET:O	1:A:312:SER:CB	2.63	0.47
1:B:296:LEU:O	1:B:300:VAL:HG23	2.14	0.47
1:B:125:ILE:HG23	1:B:129:PHE:CE1	2.49	0.47
1:A:227:GLU:OE1	2:C:141:ARG:HD2	2.14	0.47
2:D:199:THR:CG2	2:D:212:THR:OG1	2.63	0.47
1:A:299:ASN:C	1:A:299:ASN:ND2	2.67	0.46
1:B:236:ALA:HB3	1:B:237:PRO:CD	2.40	0.46
2:D:230:PHE:HB3	2:D:245:VAL:CG1	2.46	0.46
1:B:128:GLY:O	1:B:132:LEU:HD22	2.15	0.46
1:A:217:ARG:HG3	2:C:97:THR:O	2.15	0.46
1:A:178:LEU:HD13	1:A:178:LEU:C	2.36	0.46
1:A:214:LEU:HD11	1:A:241:LEU:HD13	1.98	0.46
1:B:95:HIS:CE1	1:B:100:THR:HG21	2.50	0.46
1:B:292:THR:O	1:B:296:LEU:HB2	2.15	0.46
1:B:117:LEU:HD22	1:B:121:PHE:CZ	2.51	0.46
1:A:17:LEU:CD2	1:A:70:LEU:HD22	2.46	0.46
2:C:49:ASP:HB3	2:C:54:ILE:HG12	1.96	0.46
2:C:14:TYR:CE2	2:C:17:GLU:HG2	2.49	0.46
1:A:21:ALA:O	1:A:24:SER:HB2	2.16	0.46
2:D:221:LEU:HD12	2:D:244:PHE:CD2	2.51	0.46
2:D:68:ILE:CG1	2:D:149:LEU:HD23	2.44	0.45
1:B:327:VAL:C	1:B:329:LYS:N	2.70	0.45
1:B:173:ASP:OD2	1:B:176:GLU:N	2.50	0.45
2:D:235:GLN:HA	2:D:239:SER:O	2.16	0.45
2:D:145:SER:O	2:D:146:GLU:HB2	2.17	0.45
1:A:186:MET:O	1:A:312:SER:OG	2.35	0.45
1:B:205:LEU:C	1:B:205:LEU:HD23	2.37	0.45
1:B:221:LEU:HD23	1:B:235:MET:SD	2.57	0.45
1:A:214:LEU:O	1:A:218:LEU:HG	2.17	0.45
1:B:285:CYS:O	1:B:289:VAL:HG23	2.17	0.45
1:A:51:ASP:N	1:A:54:GLN:HB2	2.32	0.44
1:A:329:LYS:O	1:A:329:LYS:HG3	2.16	0.44
2:D:242:THR:HG22	3:D:268:HOH:O	2.16	0.44
1:A:160:LEU:O	1:A:164:LEU:HG	2.17	0.44
1:A:200:PHE:C	1:A:203:PRO:HD2	2.38	0.44
1:B:193:ASN:HD22	1:B:195:GLU:N	2.15	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:9:ASN:H	2:C:25:ASN:ND2	2.15	0.44
1:B:120:LEU:C	1:B:120:LEU:HD23	2.38	0.44
1:B:322:LEU:HD12	1:B:325:VAL:CG2	2.48	0.44
2:D:1:MET:O	2:D:30:LYS:HE2	2.18	0.43
2:C:84:LEU:CG	2:C:110:MET:HE3	2.48	0.43
1:A:140:PHE:O	1:A:141:LYS:HB2	2.17	0.43
1:A:234:LYS:O	1:A:237:PRO:HD2	2.18	0.43
1:A:12:GLY:O	1:A:15:LEU:HB3	2.18	0.43
1:B:17:LEU:C	1:B:17:LEU:HD23	2.39	0.43
2:C:39:GLN:O	2:C:40:ASN:C	2.57	0.43
2:D:80:ALA:HB1	2:D:125:GLU:HG2	1.99	0.43
2:C:203:ASN:HB2	2:C:224:LEU:CD1	2.49	0.43
1:A:51:ASP:N	1:A:54:GLN:N	2.67	0.42
2:D:201:LEU:HD22	2:D:224:LEU:HD22	1.99	0.42
2:C:26:PHE:HB2	2:C:209:PHE:CZ	2.55	0.42
1:B:176:GLU:HA	1:B:176:GLU:OE1	2.20	0.42
2:C:152:LEU:O	2:C:184:PHE:HA	2.20	0.42
2:C:201:LEU:O	2:C:207:PHE:HA	2.20	0.42
1:A:214:LEU:HD11	1:A:241:LEU:CD1	2.50	0.42
2:C:85:ASP:O	2:C:89:MET:HG3	2.19	0.42
1:B:63:LEU:N	1:B:64:PRO:CD	2.82	0.42
1:B:21:ALA:HA	1:B:295:LEU:HD21	2.01	0.42
1:B:66:ILE:O	1:B:70:LEU:HG	2.19	0.42
1:B:122:THR:O	1:B:126:LEU:HB2	2.19	0.42
2:C:232:GLN:HB3	2:C:232:GLN:HE21	1.55	0.42
2:D:205:GLN:HG2	3:D:371:HOH:O	2.20	0.42
1:A:51:ASP:HB3	1:A:54:GLN:NE2	2.35	0.42
2:D:163:ASN:HA	2:D:163:ASN:HD22	1.70	0.41
1:A:97:ILE:HG13	1:A:99:VAL:HG12	2.01	0.41
1:A:21:ALA:HA	1:A:295:LEU:HD21	2.01	0.41
1:A:253:GLN:HB3	1:A:253:GLN:HE21	1.72	0.41
1:B:229:LYS:O	1:B:229:LYS:HD3	2.20	0.41
2:D:28:LEU:HD21	2:D:34:LEU:HG	2.01	0.41
2:C:104:HIS:O	2:C:107:GLN:HB3	2.21	0.41
1:B:129:PHE:O	1:B:132:LEU:HB2	2.21	0.41
1:B:97:ILE:O	1:B:97:ILE:HG13	2.20	0.41
2:D:199:THR:HG22	2:D:212:THR:OG1	2.20	0.41
1:B:62:ARG:NH2	1:B:62:ARG:HG3	2.30	0.41
2:D:190:ASN:ND2	2:D:243:HIS:CE1	2.88	0.41
1:B:215:SER:HB3	2:D:100:LYS:HE3	2.02	0.41
1:B:132:LEU:HB3	1:B:244:PHE:CE2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:117:LEU:C	1:A:117:LEU:HD13	2.41	0.41
1:B:215:SER:HB2	2:D:100:LYS:HE3	2.01	0.41
1:A:93:ASN:C	1:A:95:HIS:H	2.23	0.41
2:C:199:THR:CG2	2:C:212:THR:OG1	2.69	0.41
2:D:201:LEU:O	2:D:207:PHE:HA	2.21	0.41
1:B:57:VAL:C	1:B:59:PHE:H	2.24	0.41
2:D:237:LYS:O	2:D:238:GLU:CG	2.68	0.40
2:D:204:LYS:HB3	2:D:204:LYS:HE2	1.93	0.40
1:B:269:HIS:HD2	1:B:326:LEU:HG	1.86	0.40
2:C:17:GLU:OE2	2:C:17:GLU:HA	2.21	0.40
1:A:160:LEU:HA	1:A:160:LEU:HD12	1.95	0.40
1:A:283:LEU:N	1:A:284:PRO:HD2	2.36	0.40
1:B:269:HIS:HB2	3:B:373:HOH:O	2.21	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	302/337 (90%)	288 (95%)	11 (4%)	3 (1%)	19 28
1	B	294/337 (87%)	276 (94%)	16 (5%)	2 (1%)	26 38
2	C	249/253 (98%)	234 (94%)	10 (4%)	5 (2%)	9 11
2	D	244/253 (96%)	234 (96%)	10 (4%)	0	100 100
All	All	1089/1180 (92%)	1032 (95%)	47 (4%)	10 (1%)	21 30

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	187	GLY
2	C	40	ASN

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Mol	Chain	Res	Type
2	C	204	LYS
2	C	205	GLN
1	B	31	SER
2	C	26	PHE
2	C	120	HIS
1	B	59	PHE
1	A	34	VAL
1	A	94	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	261/284 (92%)	244 (94%)	17 (6%)	21	33
1	B	247/284 (87%)	231 (94%)	16 (6%)	21	33
2	C	221/223 (99%)	208 (94%)	13 (6%)	24	38
2	D	218/223 (98%)	204 (94%)	14 (6%)	22	34
All	All	947/1014 (93%)	887 (94%)	60 (6%)	22	35

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	78	LEU
1	A	89	ASN
1	A	93	ASN
1	A	126	LEU
1	A	147	LEU
1	A	160	LEU
1	A	167	LEU
1	A	177	LYS
1	A	197	LEU
1	A	206	LEU
1	A	221	LEU
1	A	223	LEU
1	A	224	ASP

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Mol	Chain	Res	Type
1	A	241	LEU
1	A	253	GLN
1	A	282	LEU
1	A	299	ASN
2	C	19	PHE
2	C	20	LEU
2	C	24	LEU
2	C	27	ASP
2	C	47	LEU
2	C	84	LEU
2	C	121	LEU
2	C	141	ARG
2	C	172	ILE
2	C	199	THR
2	C	200	LEU
2	C	232	GLN
2	C	245	VAL
1	B	78	LEU
1	B	89	ASN
1	B	117	LEU
1	B	193	ASN
1	B	215	SER
1	B	217	ARG
1	B	223	LEU
1	B	224	ASP
1	B	241	LEU
1	B	253	GLN
1	B	265	LEU
1	B	282	LEU
1	B	283	LEU
1	B	296	LEU
1	B	306	ASP
1	B	330	LEU
2	D	7	VAL
2	D	24	LEU
2	D	34	LEU
2	D	37	LEU
2	D	47	LEU
2	D	121	LEU
2	D	124	ARG
2	D	199	THR
2	D	206	ASN

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Mol	Chain	Res	Type
2	D	238	GLU
2	D	240	PHE
2	D	242	THR
2	D	247	LEU
2	D	251	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (48) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	54	GLN
1	A	55	GLN
1	A	60	GLN
1	A	89	ASN
1	A	93	ASN
1	A	95	HIS
1	A	169	GLN
1	A	253	GLN
1	A	269	HIS
1	A	280	GLN
1	A	299	ASN
2	C	9	ASN
2	C	25	ASN
2	C	73	GLN
2	C	96	ASN
2	C	163	ASN
2	C	176	GLN
2	C	178	GLN
2	C	179	ASN
2	C	187	HIS
2	C	190	ASN
2	C	206	ASN
2	C	220	ASN
2	C	232	GLN
1	B	84	GLN
1	B	89	ASN
1	B	169	GLN
1	B	193	ASN
1	B	253	GLN
1	B	269	HIS
1	B	278	ASN
1	B	299	ASN
2	D	9	ASN

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Mol	Chain	Res	Type
2	D	15	GLN
2	D	25	ASN
2	D	29	ASN
2	D	55	HIS
2	D	59	GLN
2	D	73	GLN
2	D	96	ASN
2	D	107	GLN
2	D	163	ASN
2	D	176	GLN
2	D	178	GLN
2	D	188	GLN
2	D	191	GLN
2	D	220	ASN
2	D	226	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

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

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	308/337 (91%)	-0.03	14 (4%)	37	38	37, 53, 86, 106	30 (9%)
1	B	300/337 (89%)	-0.07	12 (4%)	42	43	28, 51, 86, 111	29 (9%)
2	C	251/253 (99%)	-0.10	11 (4%)	38	39	23, 42, 67, 80	17 (6%)
2	D	248/253 (98%)	-0.20	11 (4%)	38	39	19, 36, 71, 95	16 (6%)
All	All	1107/1180 (93%)	-0.09	48 (4%)	39	40	19, 47, 79, 111	92 (8%)

All (48) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	330	LEU	7.6
2	D	240	PHE	5.4
2	D	15	GLN	5.3
1	B	11	PHE	4.9
2	C	204	LYS	4.8
1	A	304	LEU	4.6
1	A	141	LYS	4.5
1	A	11	PHE	4.1
2	C	16	ALA	3.8
2	D	16	ALA	3.8
1	B	118	TYR	3.6
1	B	55	GLN	3.6
2	C	18	ASN	3.6
2	D	239	SER	3.5
1	A	140	PHE	3.5
1	B	7	PRO	3.4
2	D	236	TYR	3.3
1	A	118	TYR	3.2
1	A	330	LEU	3.2
1	A	7	PRO	3.2
1	A	307	ALA	3.1

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Mol	Chain	Res	Type	RSRZ
2	D	14	TYR	3.1
1	B	56	GLN	3.1
1	A	6	TYR	3.0
2	D	13	TYR	2.9
1	A	328	TYR	2.8
2	C	41	GLY	2.8
1	B	6	TYR	2.7
1	A	8	LYS	2.7
2	C	103	SER	2.6
1	A	306	ASP	2.6
1	B	176	GLU	2.6
2	C	40	ASN	2.6
2	D	56	ARG	2.5
2	C	205	GLN	2.4
2	C	17	GLU	2.4
1	A	176	GLU	2.3
1	A	114	GLY	2.3
2	D	235	GLN	2.3
2	D	213	ARG	2.3
1	B	175	GLU	2.2
1	B	30	TYR	2.2
1	B	54	GLN	2.1
2	C	15	GLN	2.1
2	D	238	GLU	2.1
2	C	89	MET	2.0
2	C	96	ASN	2.0
1	B	244	PHE	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)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.