Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 09:36 PM GMT

PDB ID	:	1PTW
Title	:	The Crystal Structure of AMP-Bound PDE4 Suggests a Mechanism for Phosphodiesterase Catalysis
Authors	:	Huai, Q.; Colicelli, J.; Ke, H.
Deposited on	:	2003-06-23
Resolution	:	2.30 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:

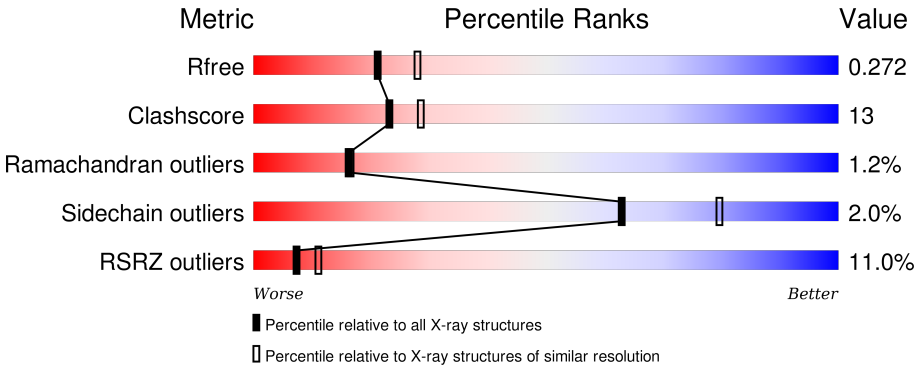
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.30 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	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (2.30-2.30)

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	360	9% 68% 23% • 7%
1	B	360	12% 60% 30% • 9%
1	C	360	11% 60% 29% • 9%
1	D	360	8% 66% 25% • 7%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 10888 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.

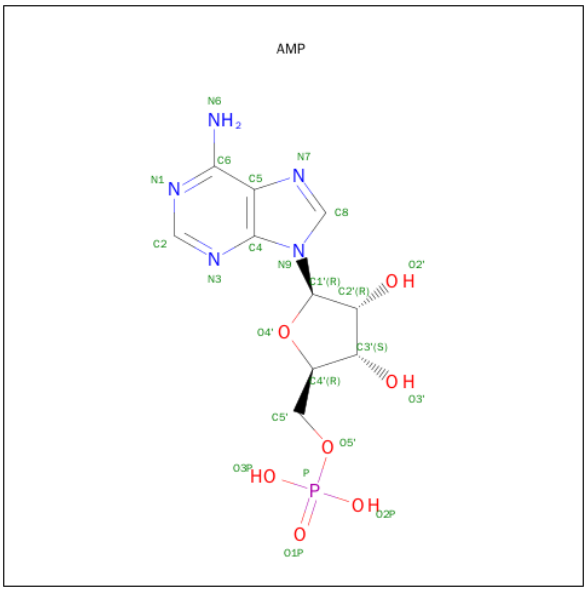
- Molecule 1 is a protein called cAMP-specific phosphodiesterase PDE4D2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	334	Total	C	N	O	S	0	0	0
			2704	1712	463	515	14			
1	B	327	Total	C	N	O	S	0	0	0
			2647	1673	452	508	14			
1	C	327	Total	C	N	O	S	0	0	0
			2647	1673	452	508	14			
1	D	334	Total	C	N	O	S	0	0	0
			2704	1712	463	515	14			

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	2	Total	Zn	0	0
			2	2		
2	A	2	Total	Zn	0	0
			2	2		
2	D	2	Total	Zn	0	0
			2	2		
2	C	2	Total	Zn	0	0
			2	2		

- Molecule 3 is ADENOSINE MONOPHOSPHATE (three-letter code: AMP) (formula: $C_{10}H_{14}N_5O_7P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
3	B	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
3	C	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
3	D	1	Total	C	N	O	P	0	0
			23	10	5	7	1		

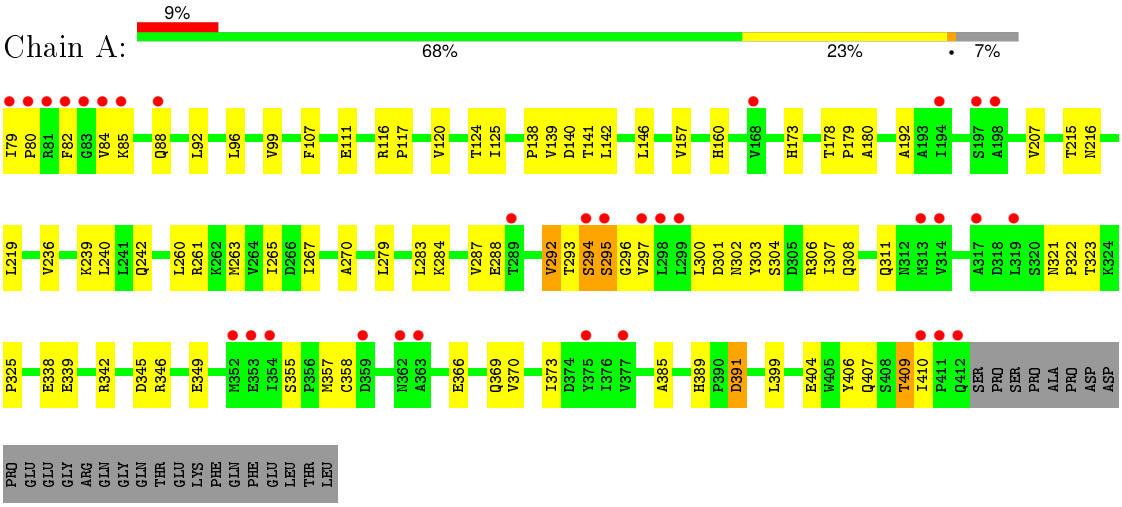
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	26	Total	O	0	0
			26	26		
4	B	13	Total	O	0	0
			13	13		
4	C	16	Total	O	0	0
			16	16		
4	D	31	Total	O	0	0
			31	31		

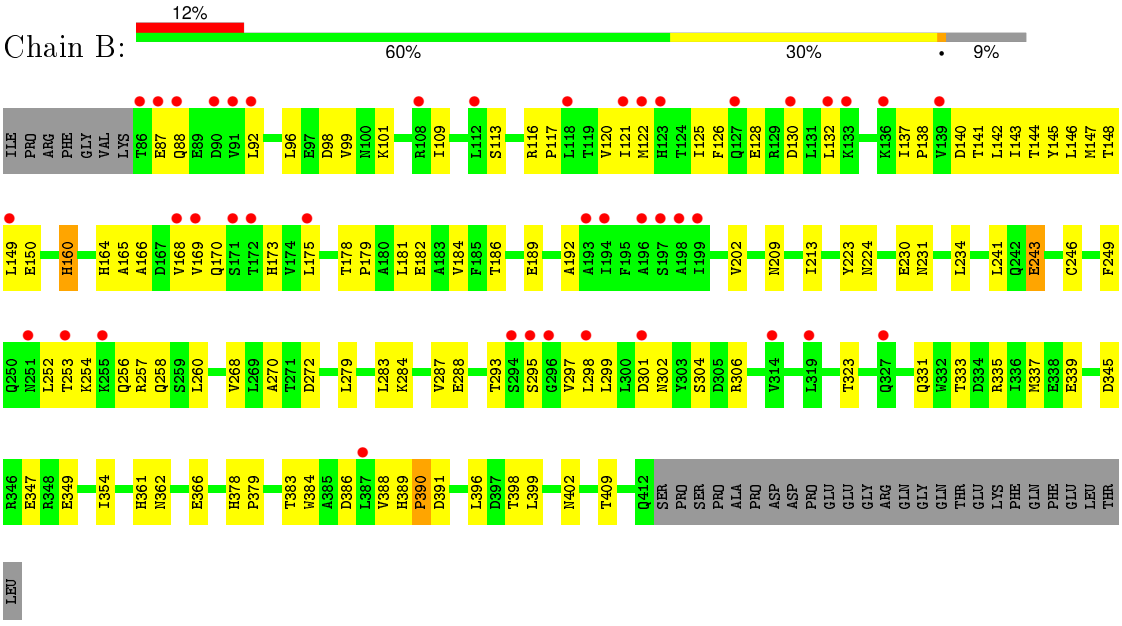
3 Residue-property plots (i)

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: cAMP-specific phosphodiesterase PDE4D2

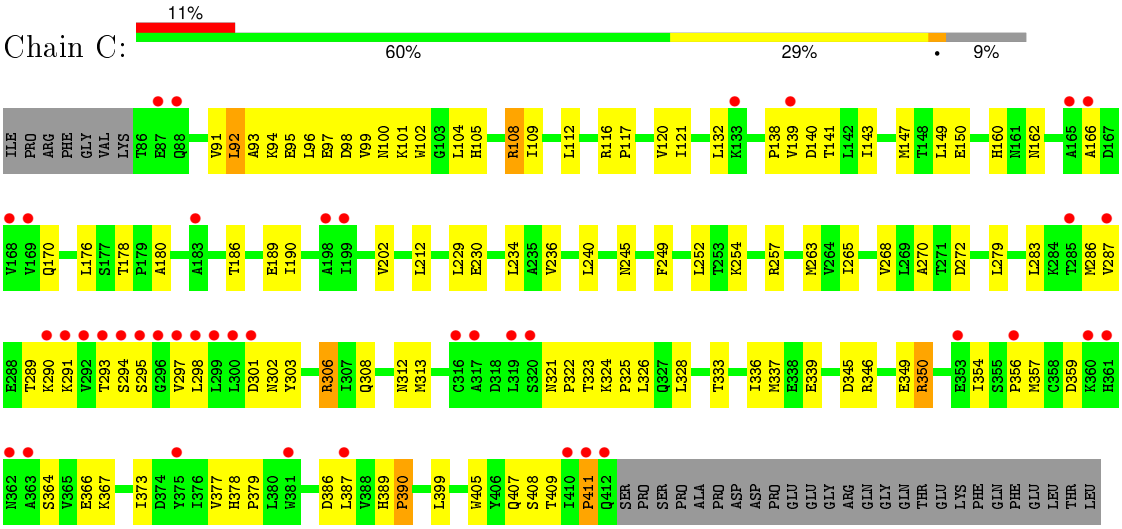


- Molecule 1: cAMP-specific phosphodiesterase PDE4D2



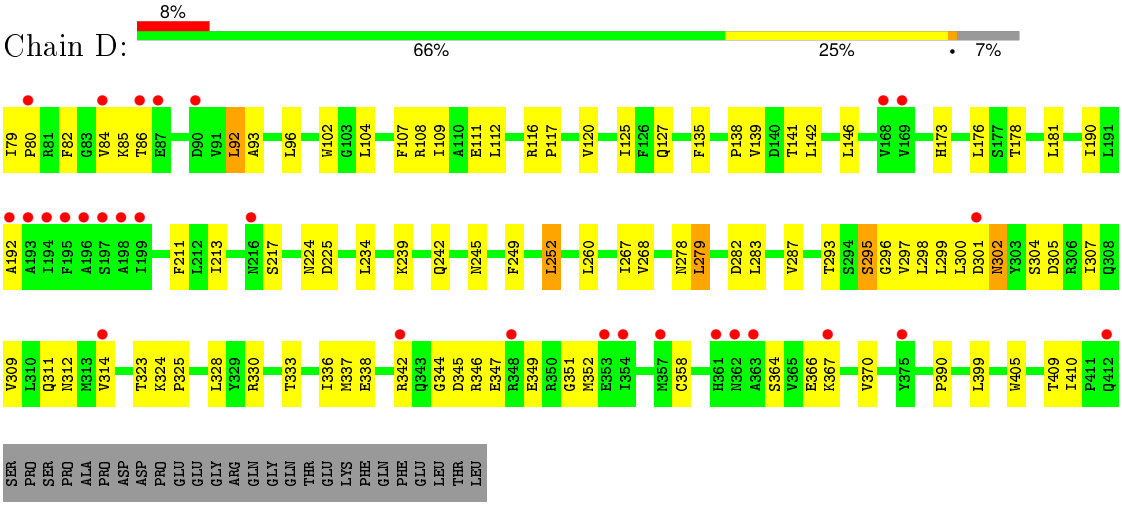
- Molecule 1: cAMP-specific phosphodiesterase PDE4D2

Chain C:



• Molecule 1: cAMP-specific phosphodiesterase PDE4D2

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	99.21Å 111.23Å 159.65Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	99.00 – 2.30 30.82 – 2.30	Depositor EDS
% Data completeness (in resolution range)	84.9 (99.00-2.30) 84.7 (30.82-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	1.50 (at 2.29Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.229 , 0.274 0.229 , 0.272	Depositor DCC
R_{free} test set	6797 reflections (10.13%)	DCC
Wilson B-factor (Å^2)	39.1	Xtriage
Anisotropy	0.131	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 41.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 70964 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	10888	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 3.20% 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

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

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	0.37	0/2760	0.61	0/3749
1	B	0.34	0/2701	0.54	0/3670
1	C	0.33	0/2701	0.54	0/3670
1	D	0.38	0/2760	0.59	1/3749 (0.0%)
All	All	0.36	0/10922	0.57	1/14838 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	252	LEU	CA-CB-CG	5.17	127.19	115.30

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	2704	0	2664	62	0
1	B	2647	0	2599	79	0
1	C	2647	0	2599	83	0
1	D	2704	0	2664	68	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	2	0	0	0	0
2	D	2	0	0	0	0
3	A	23	0	12	1	0
3	B	23	0	12	1	0
3	C	23	0	12	2	0
3	D	23	0	12	0	0
4	A	26	0	0	1	0
4	B	13	0	0	0	0
4	C	16	0	0	0	0
4	D	31	0	0	0	0
All	All	10888	0	10574	286	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 13.

All (286) 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:292:VAL:HG12	1:A:293:THR:H	1.15	1.04
1:C:306:ARG:HH11	1:C:306:ARG:HB3	1.23	1.03
1:D:302:ASN:HD22	1:D:302:ASN:H	1.15	0.88
1:C:306:ARG:CB	1:C:306:ARG:HH11	1.98	0.77
1:C:290:LYS:HE3	1:C:298:LEU:HD21	1.67	0.77
1:C:293:THR:HG22	1:C:294:SER:H	1.48	0.77
1:C:325:PRO:HD2	1:C:328:LEU:HD12	1.68	0.76
1:A:345:ASP:O	1:A:349:GLU:HG3	1.87	0.74
1:B:270:ALA:HB1	1:B:279:LEU:HD11	1.71	0.73
1:A:292:VAL:HG12	1:A:293:THR:N	1.98	0.72
1:D:366:GLU:HG2	1:D:409:THR:HB	1.71	0.72
1:D:338:GLU:O	1:D:342:ARG:HG2	1.90	0.72
1:A:346:ARG:HA	1:A:349:GLU:OE1	1.89	0.71
1:B:254:LYS:O	1:B:258:GLN:HG3	1.91	0.70
1:B:178:THR:HG23	1:B:181:LEU:HB2	1.74	0.70
1:B:87:GLU:HG3	1:B:88:GLN:H	1.57	0.70
1:C:104:LEU:HD11	1:C:109:ILE:HD11	1.75	0.69
1:D:79:ILE:N	1:D:80:PRO:HD2	2.08	0.68
1:C:143:ILE:O	1:C:147:MET:HG3	1.94	0.68
1:B:378:HIS:HB3	1:B:379:PRO:HD3	1.75	0.67
1:C:293:THR:HG22	1:C:294:SER:N	2.10	0.67
1:C:234:LEU:HD21	1:C:268:VAL:HB	1.77	0.67
1:D:302:ASN:ND2	1:D:302:ASN:H	1.91	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:302:ASN:HD22	1:D:302:ASN:N	1.90	0.66
1:D:84:VAL:HG12	1:D:85:LYS:H	1.60	0.66
1:B:230:GLU:HG2	1:B:272:ASP:HB2	1.78	0.66
1:B:345:ASP:O	1:B:349:GLU:HG3	1.95	0.65
1:A:96:LEU:O	1:A:99:VAL:HG23	1.96	0.65
1:C:354:ILE:HG21	1:C:359:ASP:HB2	1.79	0.64
1:B:87:GLU:HG3	1:B:88:GLN:N	2.12	0.63
1:B:116:ARG:HD3	1:B:150:GLU:OE1	1.98	0.63
1:C:302:ASN:O	1:C:306:ARG:HG3	1.99	0.62
1:B:323:THR:HG22	1:B:399:LEU:HD13	1.82	0.62
1:A:284:LYS:O	1:A:288:GLU:HG3	1.99	0.62
1:B:144:THR:HG22	1:B:246:CYS:SG	2.40	0.62
1:D:84:VAL:HG12	1:D:85:LYS:N	2.15	0.61
1:A:180:ALA:O	1:A:297:VAL:HG13	2.00	0.61
1:B:178:THR:HG21	1:B:181:LEU:HD12	1.82	0.61
1:B:253:THR:OG1	1:B:256:GLN:HG3	2.01	0.61
1:A:307:ILE:O	1:A:311:GLN:HG3	2.02	0.60
1:B:142:LEU:O	1:B:146:LEU:HG	2.01	0.60
1:C:236:VAL:O	1:C:240:LEU:HG	2.02	0.59
1:C:286:MET:HE1	1:C:308:GLN:HB3	1.84	0.59
1:C:102:TRP:NE1	1:C:324:LYS:HD3	2.17	0.59
1:C:270:ALA:HB1	1:C:279:LEU:HD11	1.84	0.58
1:A:96:LEU:O	1:A:99:VAL:CG2	2.51	0.58
1:A:239:LYS:NZ	1:D:239:LYS:NZ	2.52	0.58
1:B:122:MET:SD	1:B:169:VAL:HG11	2.44	0.57
1:A:79:ILE:N	1:A:80:PRO:HD2	2.18	0.57
1:A:82:PHE:O	1:A:84:VAL:HG23	2.05	0.57
1:C:116:ARG:HE	1:C:147:MET:HE2	1.69	0.57
1:C:287:VAL:HG22	1:C:387:LEU:HD13	1.87	0.57
1:D:302:ASN:OD1	1:D:304:SER:HB3	2.05	0.57
1:B:175:LEU:O	1:B:178:THR:HG22	2.06	0.56
1:D:79:ILE:N	1:D:79:ILE:HD12	2.20	0.56
1:A:160:HIS:ND1	1:A:339:GLU:OE2	2.29	0.56
1:C:373:ILE:HA	1:C:377:VAL:HB	1.88	0.56
1:D:213:ILE:HG23	1:D:225:ASP:OD1	2.06	0.55
1:B:143:ILE:O	1:B:147:MET:HG3	2.06	0.55
1:B:165:ALA:O	1:B:169:VAL:HG23	2.06	0.55
1:A:302:ASN:O	1:A:306:ARG:HG3	2.07	0.55
1:A:79:ILE:N	1:A:80:PRO:CD	2.69	0.55
1:D:142:LEU:O	1:D:146:LEU:HG	2.07	0.55
1:A:304:SER:O	1:A:308:GLN:HB2	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:234:LEU:HD21	1:B:268:VAL:HB	1.89	0.55
1:B:361:HIS:C	1:B:362:ASN:HD22	2.10	0.54
1:D:344:GLY:HA3	1:D:358:CYS:O	2.07	0.54
1:B:383:THR:O	1:B:386:ASP:HB2	2.08	0.54
1:C:306:ARG:NH1	1:C:306:ARG:HB3	2.07	0.54
1:A:192:ALA:HB2	1:A:260:LEU:HD12	1.90	0.54
1:C:230:GLU:HG2	1:C:272:ASP:HB2	1.90	0.54
1:C:409:THR:O	1:C:411:PRO:HD3	2.07	0.54
1:B:331:GLN:O	1:B:335:ARG:HG3	2.08	0.54
1:B:178:THR:CG2	1:B:181:LEU:HD12	2.38	0.54
1:C:121:ILE:HD12	1:C:166:ALA:HB1	1.90	0.54
3:C:509:AMP:H3'	3:C:509:AMP:O1P	2.08	0.53
1:C:120:VAL:HG23	1:C:121:ILE:N	2.23	0.53
1:B:409:THR:O	1:B:409:THR:HG22	2.08	0.53
1:D:104:LEU:HD11	1:D:109:ILE:HD11	1.90	0.53
1:D:370:VAL:HG21	1:D:410:ILE:HD11	1.91	0.53
1:A:242:GLN:OE1	1:D:242:GLN:OE1	2.27	0.53
1:D:345:ASP:O	1:D:349:GLU:HG3	2.08	0.53
1:B:284:LYS:HE2	1:B:383:THR:OG1	2.09	0.53
1:A:366:GLU:HG2	1:A:409:THR:HG22	1.91	0.53
1:C:378:HIS:HB3	1:C:379:PRO:HD3	1.91	0.53
1:B:96:LEU:O	1:B:99:VAL:HG23	2.09	0.52
1:C:139:VAL:HG23	1:C:140:ASP:N	2.23	0.52
1:B:116:ARG:NH2	1:D:349:GLU:OE1	2.43	0.52
1:D:295:SER:O	1:D:297:VAL:N	2.40	0.52
1:C:263:MET:HG2	1:C:303:TYR:OH	2.10	0.52
1:B:302:ASN:O	1:B:306:ARG:HG3	2.09	0.52
1:A:142:LEU:O	1:A:146:LEU:HG	2.10	0.52
1:D:330:ARG:HH11	1:D:405:TRP:HH2	1.57	0.52
1:C:356:PRO:O	1:C:357:MET:HB2	2.10	0.52
1:D:346:ARG:HA	1:D:349:GLU:OE1	2.10	0.51
1:A:292:VAL:CG1	1:A:293:THR:H	1.92	0.51
1:A:349:GLU:HB3	1:C:147:MET:SD	2.51	0.51
1:D:96:LEU:HD11	1:D:120:VAL:CG1	2.40	0.51
1:A:292:VAL:CG1	1:A:293:THR:N	2.67	0.51
1:A:338:GLU:OE2	1:A:342:ARG:NH2	2.44	0.51
1:D:181:LEU:HD21	1:D:298:LEU:HD22	1.93	0.51
1:C:336:ILE:HG23	1:C:337:MET:N	2.26	0.51
1:B:121:ILE:HG21	1:B:170:GLN:HB2	1.93	0.50
1:C:254:LYS:HD2	1:C:257:ARG:HH12	1.75	0.50
1:C:321:ASN:CG	1:C:322:PRO:HD3	2.32	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:345:ASP:O	1:C:349:GLU:HG3	2.10	0.50
1:C:407:GLN:C	1:C:409:THR:H	2.15	0.50
1:D:279:LEU:HD22	1:D:312:ASN:OD1	2.11	0.50
1:A:404:GLU:O	1:A:407:GLN:N	2.45	0.50
1:D:249:PHE:CZ	1:D:260:LEU:HD21	2.46	0.50
1:B:92:LEU:HD23	1:B:92:LEU:O	2.11	0.50
1:A:406:TYR:O	1:A:410:ILE:HG13	2.12	0.50
1:A:321:ASN:CG	1:A:322:PRO:HD3	2.32	0.50
1:A:366:GLU:O	1:A:370:VAL:HG23	2.12	0.50
1:B:145:TYR:CE1	1:B:241:LEU:HD23	2.47	0.50
1:C:94:LYS:HA	1:C:97:GLU:OE2	2.12	0.50
1:A:300:LEU:HD13	1:A:306:ARG:HA	1.93	0.49
1:B:178:THR:CG2	1:B:181:LEU:HB2	2.42	0.49
1:C:333:THR:O	1:C:336:ILE:HG22	2.12	0.49
1:B:366:GLU:HG2	1:B:409:THR:CG2	2.43	0.49
1:C:93:ALA:O	1:C:97:GLU:HG3	2.13	0.49
1:A:270:ALA:HB1	1:A:279:LEU:HD11	1.93	0.49
1:B:186:THR:OG1	1:B:189:GLU:HG3	2.12	0.49
1:C:308:GLN:O	1:C:312:ASN:ND2	2.41	0.49
1:D:141:THR:HG23	1:D:245:ASN:O	2.13	0.49
1:B:148:THR:HG21	1:B:243:GLU:HG3	1.94	0.49
1:D:302:ASN:ND2	1:D:302:ASN:N	2.54	0.49
1:B:109:ILE:O	1:B:113:SER:HB3	2.13	0.49
1:D:192:ALA:HB2	1:D:260:LEU:HD12	1.95	0.49
1:B:302:ASN:OD1	1:B:304:SER:HB3	2.13	0.49
1:C:346:ARG:O	1:C:350:ARG:HD2	2.13	0.48
1:D:127:GLN:HE21	1:D:127:GLN:HA	1.79	0.48
1:C:116:ARG:HH11	1:C:116:ARG:HG2	1.78	0.48
1:D:307:ILE:O	1:D:311:GLN:HG3	2.14	0.48
1:B:120:VAL:HG23	1:B:121:ILE:N	2.29	0.48
1:B:366:GLU:HG2	1:B:409:THR:HB	1.95	0.47
1:C:212:LEU:HD11	1:C:229:LEU:HD21	1.96	0.47
1:C:336:ILE:CG2	1:C:337:MET:N	2.76	0.47
1:D:138:PRO:HG2	1:D:141:THR:OG1	2.15	0.47
1:C:326:LEU:HD21	1:C:405:TRP:CE2	2.48	0.47
1:C:293:THR:CG2	1:C:294:SER:H	2.24	0.47
1:A:215:THR:O	1:A:216:ASN:HB2	2.14	0.47
1:A:236:VAL:O	1:A:240:LEU:HG	2.15	0.47
1:C:160:HIS:NE2	3:C:509:AMP:O1P	2.37	0.47
1:D:300:LEU:HD11	1:D:309:VAL:HG21	1.96	0.47
1:D:234:LEU:HD21	1:D:268:VAL:HB	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:160:HIS:ND1	1:C:339:GLU:OE2	2.48	0.47
1:B:333:THR:O	1:B:337:MET:HG2	2.15	0.47
1:D:333:THR:O	1:D:337:MET:HG2	2.15	0.47
1:B:192:ALA:HB2	1:B:260:LEU:HD12	1.97	0.47
1:B:160:HIS:ND1	1:B:339:GLU:OE2	2.42	0.47
1:B:132:LEU:HA	1:B:137:ILE:HB	1.96	0.46
1:A:179:PRO:HD2	1:A:391:ASP:OD2	2.15	0.46
1:B:249:PHE:HA	1:B:252:LEU:HD13	1.97	0.46
1:B:179:PRO:O	1:B:182:GLU:HB2	2.14	0.46
1:A:116:ARG:N	1:A:117:PRO:CD	2.78	0.46
1:A:157:VAL:HG13	1:A:339:GLU:OE1	2.15	0.46
1:B:283:LEU:O	1:B:287:VAL:HG23	2.16	0.46
1:D:104:LEU:HD11	1:D:109:ILE:CD1	2.46	0.46
1:C:289:THR:HG22	1:C:289:THR:O	2.16	0.46
1:C:323:THR:HG22	1:C:399:LEU:HD13	1.97	0.46
1:D:333:THR:HA	1:D:336:ILE:HG22	1.97	0.46
1:D:364:SER:HB3	1:D:367:LYS:HB3	1.97	0.46
1:A:207:VAL:HG13	1:A:346:ARG:HH21	1.80	0.46
1:C:104:LEU:HD12	1:C:105:HIS:H	1.80	0.46
1:D:108:ARG:CZ	1:D:112:LEU:HD21	2.46	0.46
1:C:94:LYS:HD2	1:C:97:GLU:OE2	2.16	0.46
1:A:283:LEU:O	1:A:287:VAL:HG23	2.16	0.45
1:B:243:GLU:OE2	1:D:217:SER:HA	2.17	0.45
1:D:323:THR:HG22	1:D:399:LEU:HD13	1.99	0.45
1:C:306:ARG:HH11	1:C:306:ARG:CG	2.29	0.45
1:B:398:THR:HG22	1:B:402:ASN:ND2	2.31	0.45
1:B:252:LEU:HA	1:B:256:GLN:OE1	2.16	0.45
1:D:301:ASP:C	1:D:301:ASP:OD2	2.54	0.45
1:C:176:LEU:HD23	1:C:313:MET:SD	2.57	0.45
1:D:135:PHE:CD1	1:D:252:LEU:HD22	2.52	0.45
1:A:357:MET:HE1	4:A:514:HOH:O	2.16	0.45
1:A:160:HIS:NE2	3:A:507:AMP:O2P	2.50	0.45
1:B:295:SER:OG	1:B:297:VAL:HG23	2.17	0.45
1:B:98:ASP:OD1	1:B:101:LYS:HD2	2.17	0.45
1:A:207:VAL:HG13	1:A:346:ARG:NH2	2.32	0.44
1:C:116:ARG:N	1:C:117:PRO:CD	2.79	0.44
1:A:369:GLN:O	1:A:373:ILE:HG13	2.16	0.44
1:C:283:LEU:O	1:C:287:VAL:HG23	2.17	0.44
1:B:116:ARG:N	1:B:117:PRO:CD	2.81	0.44
1:B:284:LYS:O	1:B:288:GLU:HG3	2.17	0.44
1:B:223:TYR:CE1	1:B:231:ASN:HB3	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:366:GLU:CD	1:C:366:GLU:H	2.20	0.44
1:D:325:PRO:HD2	1:D:328:LEU:HD12	2.00	0.44
1:C:249:PHE:HB3	1:C:252:LEU:HD12	2.00	0.44
1:C:139:VAL:CG2	1:C:140:ASP:N	2.81	0.44
3:B:508:AMP:O1P	3:B:508:AMP:H3'	2.17	0.44
1:B:138:PRO:HG2	1:B:141:THR:HB	2.00	0.44
1:C:104:LEU:HD23	1:C:170:GLN:HG3	1.99	0.43
1:B:137:ILE:CG2	1:B:142:LEU:HB2	2.48	0.43
1:D:82:PHE:CZ	1:D:93:ALA:HA	2.53	0.43
1:D:181:LEU:CD2	1:D:298:LEU:HD22	2.48	0.43
1:B:396:LEU:HD23	1:B:396:LEU:O	2.17	0.43
1:D:107:PHE:O	1:D:111:GLU:HG3	2.18	0.43
1:A:265:ILE:HD13	1:B:224:ASN:O	2.18	0.43
1:B:362:ASN:HD22	1:B:362:ASN:N	2.15	0.43
1:B:99:VAL:O	1:B:170:GLN:NE2	2.50	0.43
1:D:108:ARG:O	1:D:112:LEU:HG	2.17	0.43
1:A:107:PHE:O	1:A:111:GLU:HG3	2.18	0.43
1:B:209:ASN:O	1:B:213:ILE:HG13	2.17	0.43
1:A:293:THR:O	1:A:294:SER:CB	2.66	0.43
1:D:305:ASP:O	1:D:309:VAL:HG23	2.17	0.43
1:D:116:ARG:N	1:D:117:PRO:CD	2.82	0.43
1:A:116:ARG:O	1:A:120:VAL:HG22	2.18	0.43
1:C:364:SER:HB3	1:C:367:LYS:HD2	2.01	0.43
1:A:125:ILE:HD13	1:A:173:HIS:HB2	2.01	0.43
1:B:249:PHE:CZ	1:B:260:LEU:HD21	2.53	0.43
1:B:126:PHE:HB3	1:B:132:LEU:HD11	2.00	0.43
1:C:150:GLU:HG3	1:C:162:ASN:HB3	2.01	0.43
1:A:385:ALA:O	1:A:389:HIS:HB2	2.19	0.43
1:C:132:LEU:HD12	1:C:132:LEU:H	1.83	0.43
1:A:139:VAL:HG23	1:A:140:ASP:N	2.34	0.43
1:B:347:GLU:OE1	1:B:354:ILE:HA	2.19	0.43
1:C:99:VAL:HG13	1:C:100:ASN:OD1	2.19	0.43
1:A:355:SER:O	1:A:358:CYS:HB2	2.19	0.43
1:D:349:GLU:C	1:D:351:GLY:H	2.22	0.42
1:C:389:HIS:HA	1:C:390:PRO:HA	1.83	0.42
1:B:181:LEU:O	1:B:184:VAL:HG23	2.19	0.42
1:C:104:LEU:HD11	1:C:109:ILE:CD1	2.46	0.42
1:D:86:THR:HG21	1:D:92:LEU:HD12	2.01	0.42
1:B:164:HIS:O	1:B:168:VAL:HG23	2.19	0.42
1:C:138:PRO:HG2	1:C:141:THR:OG1	2.20	0.42
1:C:180:ALA:O	1:C:297:VAL:HG13	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:150:GLU:HG3	1:C:162:ASN:CB	2.49	0.42
1:C:293:THR:CG2	1:C:294:SER:N	2.80	0.42
1:B:120:VAL:HG23	1:B:121:ILE:H	1.85	0.42
1:A:138:PRO:HG2	1:A:141:THR:OG1	2.20	0.42
1:B:149:LEU:HD12	1:B:202:VAL:HG21	2.01	0.42
1:A:99:VAL:HG21	1:A:124:THR:HG21	2.01	0.42
1:A:404:GLU:O	1:A:407:GLN:HB2	2.19	0.42
1:D:135:PHE:HD1	1:D:252:LEU:HD22	1.85	0.42
1:A:349:GLU:HB3	1:C:147:MET:HE1	2.01	0.42
1:D:79:ILE:N	1:D:80:PRO:CD	2.80	0.42
1:C:176:LEU:HD13	1:C:190:ILE:HG23	2.02	0.42
1:A:219:LEU:HD12	1:A:219:LEU:HA	1.89	0.42
1:C:139:VAL:O	1:C:143:ILE:HG13	2.21	0.41
1:B:113:SER:OG	1:B:116:ARG:HB2	2.19	0.41
1:A:303:TYR:O	1:A:307:ILE:HG22	2.19	0.41
1:C:289:THR:O	1:C:291:LYS:HG3	2.20	0.41
1:D:347:GLU:O	1:D:352:MET:HB2	2.20	0.41
1:C:326:LEU:HD21	1:C:405:TRP:CD2	2.56	0.41
1:D:336:ILE:HG23	1:D:337:MET:N	2.35	0.41
1:D:125:ILE:HD13	1:D:173:HIS:HB2	2.02	0.41
1:B:389:HIS:HA	1:B:390:PRO:HA	1.86	0.41
1:C:91:VAL:O	1:C:95:GLU:HG2	2.20	0.41
1:B:257:ARG:HB2	1:B:257:ARG:NH1	2.35	0.41
1:A:323:THR:HG22	1:A:399:LEU:HD13	2.03	0.41
1:A:139:VAL:HG23	1:A:140:ASP:OD1	2.21	0.41
1:C:138:PRO:HG2	1:C:141:THR:CB	2.51	0.41
1:D:283:LEU:O	1:D:287:VAL:HG23	2.20	0.41
1:D:84:VAL:CG1	1:D:85:LYS:H	2.32	0.41
1:B:306:ARG:HH11	1:B:306:ARG:HG2	1.86	0.41
1:C:108:ARG:NH1	1:C:112:LEU:HD21	2.36	0.41
1:C:92:LEU:HD22	1:C:96:LEU:HD11	2.01	0.41
1:A:293:THR:HA	1:A:296:GLY:H	1.86	0.41
1:C:230:GLU:H	1:C:230:GLU:CD	2.24	0.41
1:A:261:ARG:O	1:A:265:ILE:HG13	2.21	0.41
1:C:265:ILE:HD13	1:D:224:ASN:HB3	2.03	0.41
1:B:384:TRP:O	1:B:388:VAL:HG22	2.21	0.41
1:A:263:MET:O	1:A:267:ILE:HG13	2.20	0.41
1:A:293:THR:HB	1:A:294:SER:H	1.65	0.41
1:A:370:VAL:HG21	1:A:410:ILE:HD11	2.03	0.41
1:D:330:ARG:NH1	1:D:405:TRP:HH2	2.19	0.41
1:D:92:LEU:HD22	1:D:96:LEU:CD1	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:121:ILE:HD12	1:B:166:ALA:HB1	2.03	0.41
1:D:102:TRP:CE2	1:D:324:LYS:HE2	2.55	0.41
1:D:84:VAL:CG1	1:D:85:LYS:N	2.84	0.40
1:C:322:PRO:HG2	1:C:377:VAL:HG21	2.03	0.40
1:C:295:SER:C	1:C:297:VAL:H	2.25	0.40
1:C:186:THR:OG1	1:C:189:GLU:HG3	2.21	0.40
1:C:98:ASP:OD1	1:C:101:LYS:HD2	2.20	0.40
1:B:128:GLU:C	1:B:130:ASP:H	2.23	0.40
1:D:267:ILE:HG21	1:D:314:VAL:HG21	2.02	0.40
1:B:125:ILE:HG23	1:B:173:HIS:ND1	2.36	0.40
1:D:176:LEU:HD13	1:D:190:ILE:HG23	2.02	0.40
1:C:149:LEU:HD12	1:C:202:VAL:HG21	2.02	0.40
1:B:287:VAL:HG11	1:B:386:ASP:HB3	2.03	0.40
1:B:125:ILE:HG23	1:B:173:HIS:CE1	2.57	0.40
1:B:293:THR:HG22	1:B:299:LEU:HD23	2.04	0.40
1:D:211:PHE:CD1	1:D:211:PHE:C	2.94	0.40
1:D:293:THR:HG22	1:D:299:LEU:HD23	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	332/360 (92%)	304 (92%)	20 (6%)	8 (2%)	7 5
1	B	325/360 (90%)	287 (88%)	34 (10%)	4 (1%)	16 16
1	C	325/360 (90%)	297 (91%)	25 (8%)	3 (1%)	21 24
1	D	332/360 (92%)	311 (94%)	20 (6%)	1 (0%)	46 57
All	All	1314/1440 (91%)	1199 (91%)	99 (8%)	16 (1%)	16 16

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	160	HIS
1	B	243	GLU
1	B	301	ASP
1	A	85	LYS
1	A	301	ASP
1	A	391	ASP
1	A	294	SER
1	A	409	THR
1	A	88	GLN
1	B	140	ASP
1	C	408	SER
1	A	295	SER
1	C	301	ASP
1	D	296	GLY
1	C	411	PRO
1	A	292	VAL

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	305/328 (93%)	301 (99%)	4 (1%)	76 87
1	B	299/328 (91%)	296 (99%)	3 (1%)	82 91
1	C	299/328 (91%)	291 (97%)	8 (3%)	52 70
1	D	305/328 (93%)	296 (97%)	9 (3%)	48 65
All	All	1208/1312 (92%)	1184 (98%)	24 (2%)	63 79

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	92	LEU
1	A	178	THR
1	A	295	SER
1	A	325	PRO
1	B	298	LEU
1	B	390	PRO

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Mol	Chain	Res	Type
1	B	391	ASP
1	C	92	LEU
1	C	108	ARG
1	C	178	THR
1	C	245	ASN
1	C	306	ARG
1	C	350	ARG
1	C	386	ASP
1	C	390	PRO
1	D	92	LEU
1	D	139	VAL
1	D	178	THR
1	D	278	ASN
1	D	279	LEU
1	D	282	ASP
1	D	295	SER
1	D	302	ASN
1	D	390	PRO

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	245	ASN
1	A	312	ASN
1	A	393	GLN
1	A	407	GLN
1	B	245	ASN
1	B	308	GLN
1	B	362	ASN
1	B	369	GLN
1	C	231	ASN
1	C	242	GLN
1	C	245	ASN
1	C	308	GLN
1	C	362	ASN
1	D	123	HIS
1	D	127	GLN
1	D	216	ASN
1	D	224	ASN
1	D	245	ASN
1	D	278	ASN
1	D	302	ASN

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

Of 12 ligands modelled in this entry, 8 are monoatomic - leaving 4 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	$\#\|Z\| > 2$
3	AMP	A	507	2	20,25,25	0.79	0	22,38,38	0.80	0
3	AMP	B	508	2	20,25,25	0.79	0	22,38,38	0.77	0
3	AMP	C	509	2	20,25,25	0.77	0	22,38,38	0.88	0
3	AMP	D	510	2	20,25,25	0.75	0	22,38,38	0.87	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	AMP	A	507	2	-	0/6/26/26	0/3/3/3
3	AMP	B	508	2	-	0/6/26/26	0/3/3/3
3	AMP	C	509	2	-	0/6/26/26	0/3/3/3
3	AMP	D	510	2	-	0/6/26/26	0/3/3/3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	507	AMP	1	0
3	B	508	AMP	1	0
3	C	509	AMP	2	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	334/360 (92%)	0.51	33 (9%) 9 14	21, 41, 85, 100	0
1	B	327/360 (90%)	0.68	42 (12%) 5 7	23, 57, 84, 100	0
1	C	327/360 (90%)	0.60	41 (12%) 5 8	27, 53, 91, 100	0
1	D	334/360 (92%)	0.30	29 (8%) 13 18	21, 36, 82, 90	0
All	All	1322/1440 (91%)	0.52	145 (10%) 7 11	21, 47, 84, 100	0

All (145) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	79	ILE	16.6
1	A	82	PHE	10.5
1	C	412	GLN	10.4
1	A	80	PRO	10.3
1	B	86	THR	8.7
1	A	83	GLY	8.7
1	B	87	GLU	8.2
1	A	295	SER	7.6
1	A	294	SER	7.3
1	C	411	PRO	7.1
1	B	295	SER	7.1
1	C	295	SER	6.6
1	B	88	GLN	6.5
1	A	412	GLN	6.0
1	B	168	VAL	5.9
1	C	299	LEU	5.0
1	C	297	VAL	5.0
1	D	412	GLN	4.9
1	C	292	VAL	4.9
1	A	81	ARG	4.6
1	A	411	PRO	4.5

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Mol	Chain	Res	Type	RSRZ
1	C	294	SER	4.5
1	D	84	VAL	4.2
1	C	296	GLY	4.2
1	B	133	LYS	4.2
1	C	362	ASN	4.1
1	A	84	VAL	4.0
1	C	287	VAL	4.0
1	B	197	SER	4.0
1	A	410	ILE	4.0
1	A	353	GLU	3.9
1	D	354	ILE	3.9
1	D	362	ASN	3.9
1	B	92	LEU	3.8
1	C	363	ALA	3.7
1	D	198	ALA	3.7
1	C	301	ASP	3.7
1	D	87	GLU	3.7
1	B	172	THR	3.6
1	A	317	ALA	3.6
1	B	294	SER	3.6
1	B	193	ALA	3.6
1	A	375	TYR	3.6
1	A	168	VAL	3.5
1	B	169	VAL	3.5
1	B	196	ALA	3.5
1	D	342	ARG	3.4
1	A	354	ILE	3.4
1	C	356	PRO	3.4
1	A	352	MET	3.4
1	B	296	GLY	3.4
1	D	86	THR	3.3
1	C	168	VAL	3.3
1	C	87	GLU	3.3
1	B	90	ASP	3.3
1	A	363	ALA	3.2
1	B	301	ASP	3.2
1	C	293	THR	3.1
1	D	196	ALA	3.1
1	B	175	LEU	3.1
1	B	112	LEU	3.0
1	C	410	ILE	3.0
1	C	285	THR	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	319	LEU	3.0
1	D	361	HIS	2.9
1	D	363	ALA	2.9
1	C	360	LYS	2.9
1	D	301	ASP	2.9
1	A	198	ALA	2.9
1	B	121	ILE	2.9
1	B	319	LEU	2.9
1	B	314	VAL	2.8
1	C	298	LEU	2.8
1	B	108	ARG	2.8
1	C	320	SER	2.8
1	C	166	ALA	2.8
1	A	289	THR	2.7
1	B	127	GLN	2.7
1	D	314	VAL	2.7
1	B	91	VAL	2.7
1	B	122	MET	2.7
1	B	132	LEU	2.7
1	A	359	ASP	2.6
1	C	198	ALA	2.6
1	B	171	SER	2.6
1	A	298	LEU	2.6
1	B	136	LYS	2.6
1	B	198	ALA	2.6
1	C	319	LEU	2.6
1	D	195	PHE	2.6
1	B	327	GLN	2.5
1	D	199	ILE	2.5
1	C	353	GLU	2.5
1	D	357	MET	2.5
1	D	80	PRO	2.5
1	D	197	SER	2.5
1	D	169	VAL	2.4
1	D	168	VAL	2.4
1	B	255	LYS	2.4
1	B	118	LEU	2.4
1	A	314	VAL	2.4
1	B	194	ILE	2.3
1	C	300	LEU	2.3
1	B	298	LEU	2.3
1	C	169	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	85	LYS	2.3
1	A	299	LEU	2.3
1	D	194	ILE	2.3
1	D	367	LYS	2.3
1	D	216	ASN	2.3
1	B	253	THR	2.2
1	C	133	LYS	2.2
1	A	197	SER	2.2
1	C	381	TRP	2.2
1	A	362	ASN	2.2
1	C	290	LYS	2.2
1	C	165	ALA	2.2
1	B	251	ASN	2.2
1	C	317	ALA	2.2
1	D	353	GLU	2.2
1	C	316	CYS	2.2
1	C	387	LEU	2.1
1	B	139	VAL	2.1
1	D	193	ALA	2.1
1	A	194	ILE	2.1
1	C	291	LYS	2.1
1	C	361	HIS	2.1
1	D	348	ARG	2.1
1	D	192	ALA	2.1
1	C	199	ILE	2.1
1	D	90	ASP	2.1
1	B	130	ASP	2.1
1	A	377	VAL	2.1
1	A	313	MET	2.1
1	B	149	LEU	2.1
1	C	375	TYR	2.1
1	B	123	HIS	2.1
1	B	199	ILE	2.1
1	B	387	LEU	2.0
1	D	375	TYR	2.0
1	A	297	VAL	2.0
1	C	183	ALA	2.0
1	A	88	GLN	2.0
1	C	88	GLN	2.0
1	C	139	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 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, 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	LLDF	B-factors(Å^2)	Q<0.9
3	AMP	C	509	23/23	0.94	0.16	-0.03	57,58,60,61	0
3	AMP	A	507	23/23	0.95	0.17	-0.06	48,53,57,58	0
3	AMP	B	508	23/23	0.93	0.15	-0.10	49,56,66,66	0
2	ZN	B	501	1/1	0.99	0.13	-0.63	47,47,47,47	0
3	AMP	D	510	23/23	0.95	0.11	-0.78	49,54,62,63	0
2	ZN	D	501	1/1	0.98	0.12	-1.19	38,38,38,38	0
2	ZN	C	501	1/1	0.99	0.10	-1.73	44,44,44,44	0
2	ZN	A	501	1/1	0.99	0.13	-1.84	37,37,37,37	0
2	ZN	C	502	1/1	0.96	0.07	-1.97	67,67,67,67	0
2	ZN	A	502	1/1	0.90	0.06	-2.04	63,63,63,63	0
2	ZN	D	502	1/1	0.98	0.02	-2.98	63,63,63,63	0
2	ZN	B	502	1/1	0.98	0.05	-3.15	68,68,68,68	0

6.5 Other polymers (i)

There are no such residues in this entry.