Full wwPDB X-ray Structure Validation Report (i)

Aug 19, 2023 – 11:40 PM EDT

PDB ID	:	2H3E
Title	:	Structure of wild-type E. coli Aspartate Transcarbamoylase in the presence of N-phosphonacetyl-L-isoasparagine at 2.3A resolution
Authors	:	Eldo, J.; Cardia, J.P.; O'Day, E.M.; Xia, J.; Tsuruta, H.; Kantrowitz, E.R.
Deposited on	:	2006-05-22
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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

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

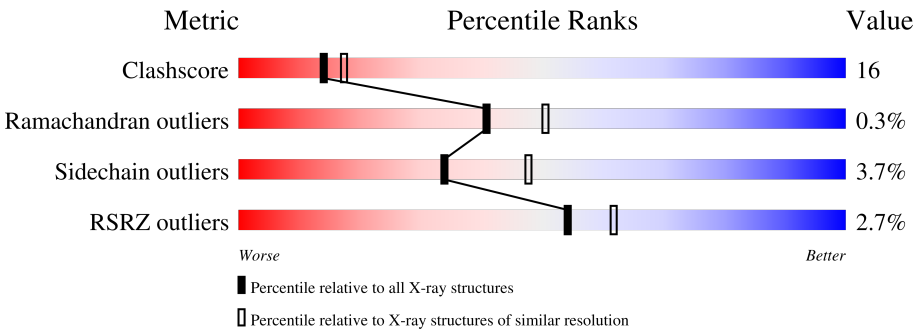
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 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))
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	310	78% 20% •
1	C	310	77% 21% •
2	B	153	7% 56% 36% • 5%
2	D	153	8% 50% 41% • 5%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 7609 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.

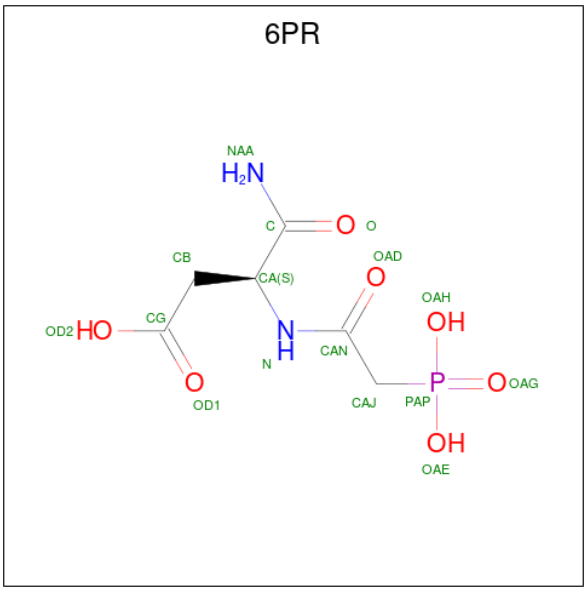
- Molecule 1 is a protein called Aspartate carbamoyltransferase catalytic chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	310	2415	1527	423	456	9	0	0	0
1	C	310	2415	1527	423	456	9	0	0	0

- Molecule 2 is a protein called Aspartate carbamoyltransferase regulatory chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	145	1134	712	200	217	5	0	0	0
2	D	145	1134	712	200	217	5	0	0	0

- Molecule 3 is (S)-4-AMINO-4-OXO-3-(2-PHOSPHONOACETAMIDO)BUTANOIC ACID (three-letter code: 6PR) (formula: $C_6H_{11}N_2O_7P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
3	A	1	16	6	2	7	1	0	0
3	C	1	16	6	2	7	1	0	0

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
4	B	1	1	1	0	0
4	D	1	1	1	0	0

- Molecule 5 is water.

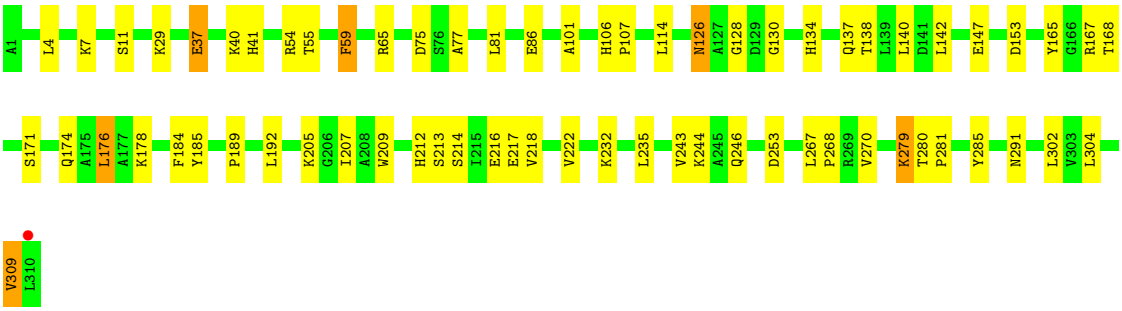
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	171	171	171	0	0
5	B	55	55	55	0	0
5	C	202	202	202	0	0
5	D	49	49	49	0	0

3 Residue-property plots (i)

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

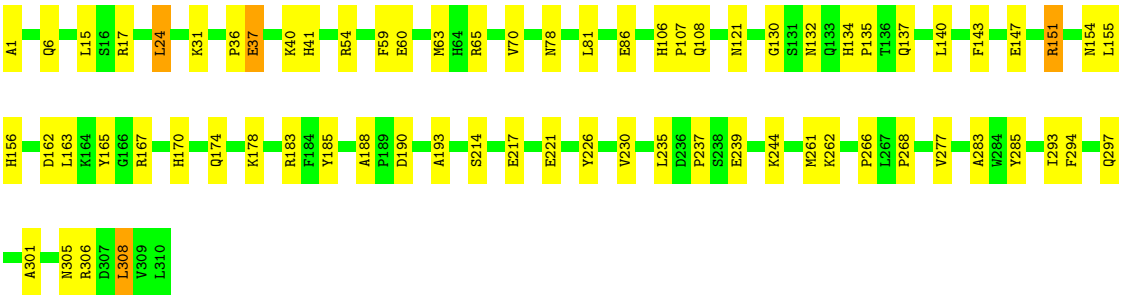
• Molecule 1: Aspartate carbamoyltransferase catalytic chain

Chain A: 78% 20% •



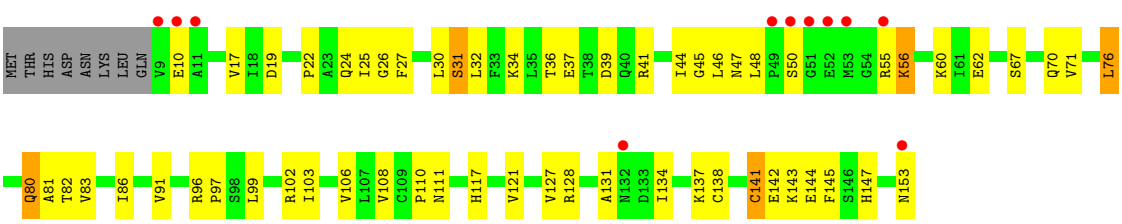
• Molecule 1: Aspartate carbamoyltransferase catalytic chain

Chain C: 77% 21% •



• Molecule 2: Aspartate carbamoyltransferase regulatory chain

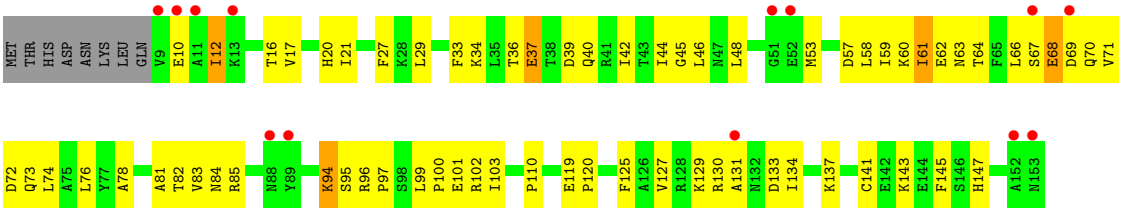
Chain B: 7% 56% 36% • 5%



• Molecule 2: Aspartate carbamoyltransferase regulatory chain

Chain D:

8%
50%
41%
5%


MET THR HIS ASP ASN LYS LEU GLN V9 E10 A11 I12 K13 T16 V17 H20 I21 F27 K28 L29 F33 K34 L35 T36 E37 T38 D39 Q40 R41 I42 T43 I44 G45 L46 N47 L48 G51 E52 M53 D57 L58 I59 K60 I61 E62 N63 T64 F65 L66 S67 E68 D69 Q70 V71
D72 Q73 L74 A75 L76 Y77 A78 A81 T82 V83 N84 R85 N88 Y89 K94 S95 R96 P97 S98 L99 P100 E101 R102 I103 P110 E119 P120 F125 A126 V127 R128 K129 R130 A131 N132 D133 I134 K137 C141 E142 K143 E144 F145 S146 H147 A152 N153

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 3 2 1	Depositor
Cell constants a, b, c, α, β, γ	120.32Å 120.32Å 154.51Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	28.41 – 2.30 28.41 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.8 (28.41-2.30) 99.8 (28.41-2.30)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.70 (at 2.31Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.206 , 0.250 0.206 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	31.9	Xtriage
Anisotropy	0.163	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 46.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.38$, $< L^2 > = 0.21$	Xtriage
Estimated twinning fraction	0.067 for -h,-k,l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	7609	wwPDB-VP
Average B, all atoms (Å^2)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.06% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

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

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: 6PR, 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	1/2461 (0.0%)	0.62	0/3339
1	C	0.39	1/2461 (0.0%)	0.63	0/3339
2	B	0.32	0/1151	0.58	0/1556
2	D	0.30	0/1151	0.59	0/1556
All	All	0.36	2/7224 (0.0%)	0.61	0/9790

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	147	GLU	CD-OE2	7.25	1.33	1.25
1	A	147	GLU	CD-OE2	6.78	1.33	1.25

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	2415	0	2422	49	0
1	C	2415	0	2422	55	0
2	B	1134	0	1151	57	0
2	D	1134	0	1151	71	0
3	A	16	0	8	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	16	0	8	2	0
4	B	1	0	0	0	0
4	D	1	0	0	0	0
5	A	171	0	0	9	1
5	B	55	0	0	7	0
5	C	202	0	0	13	0
5	D	49	0	0	9	0
All	All	7609	0	7162	225	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 16.

All (225) 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:C:167:ARG:HE	3:C:332:6PR:HAA2	1.11	0.96
2:B:138:CYS:HB3	2:B:141:CYS:HB2	1.51	0.93
1:A:167:ARG:HE	3:A:331:6PR:HAA2	1.23	0.85
2:D:20:HIS:HB3	2:D:53:MET:HE1	1.63	0.81
2:D:36:THR:HG22	5:D:187:HOH:O	1.79	0.80
1:A:126:ASN:ND2	1:A:128:GLY:H	1.82	0.77
2:D:84:ASN:OD1	2:D:94:LYS:HG2	1.86	0.76
2:D:34:LYS:HB3	2:D:37:GLU:OE1	1.88	0.73
1:C:183:ARG:HH11	1:C:183:ARG:HG2	1.54	0.72
1:C:106:HIS:HD2	1:C:108:GLN:H	1.38	0.71
2:B:36:THR:HG22	5:B:207:HOH:O	1.89	0.70
2:B:67:SER:OG	2:B:70:GLN:HG3	1.91	0.70
1:A:29:LYS:HD2	1:A:309:VAL:HG23	1.73	0.70
2:D:71:VAL:O	2:D:74:LEU:HB3	1.92	0.69
1:A:153:ASP:HB3	5:A:472:HOH:O	1.93	0.68
2:D:130:ARG:HG2	2:D:131:ALA:H	1.58	0.68
1:A:29:LYS:HD2	1:A:309:VAL:CG2	2.23	0.68
2:B:102:ARG:HA	2:B:127:VAL:HG23	1.75	0.68
2:D:45:GLY:HA3	2:D:48:LEU:HD11	1.76	0.67
1:C:106:HIS:CD2	1:C:108:GLN:H	2.13	0.67
1:C:170:HIS:O	1:C:174:GLN:HG3	1.93	0.67
1:A:137:GLN:HG2	1:A:168:THR:HG22	1.76	0.67
2:D:99:LEU:HD22	2:D:127:VAL:HG11	1.76	0.67
1:A:253:ASP:HB3	5:A:340:HOH:O	1.94	0.66
2:D:83:VAL:CG2	2:D:95:SER:HB2	2.27	0.65
1:A:130:GLY:O	1:A:167:ARG:HD3	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:138:CYS:CB	2:B:141:CYS:HB2	2.25	0.65
2:B:141:CYS:HB3	2:B:143:LYS:H	1.62	0.65
2:B:67:SER:H	2:B:70:GLN:NE2	1.94	0.65
1:C:15:LEU:O	1:C:178:LYS:HE2	1.98	0.64
1:A:167:ARG:NE	3:A:331:6PR:HAA2	1.95	0.63
2:D:12:ILE:N	2:D:12:ILE:HD13	2.14	0.62
2:D:10:GLU:HB2	2:D:60:LYS:NZ	2.15	0.62
1:C:130:GLY:O	1:C:167:ARG:HD3	2.00	0.62
2:D:40:GLN:HG3	5:D:201:HOH:O	2.00	0.61
2:D:34:LYS:O	2:D:37:GLU:HB2	2.01	0.61
2:B:143:LYS:HE2	5:B:163:HOH:O	2.00	0.61
2:B:147:HIS:HB2	5:B:203:HOH:O	2.01	0.60
1:A:171:SER:HB2	5:A:468:HOH:O	2.01	0.60
2:B:67:SER:H	2:B:70:GLN:HE21	1.49	0.60
1:C:293:ILE:HG22	1:C:297:GLN:HE21	1.66	0.60
2:D:62:GLU:HB2	5:D:191:HOH:O	2.02	0.60
2:B:99:LEU:HD11	2:B:134:ILE:HD13	1.84	0.59
2:B:17:VAL:HG13	2:B:60:LYS:HG2	1.83	0.59
1:A:54:ARG:NH1	3:A:331:6PR:OAH	2.36	0.58
2:B:134:ILE:HB	5:B:204:HOH:O	2.03	0.58
1:C:106:HIS:CD2	1:C:107:PRO:HD2	2.38	0.58
1:C:156:HIS:HD2	1:C:185:TYR:OH	1.87	0.58
1:A:218:VAL:O	1:A:222:VAL:HG13	2.04	0.58
1:A:75:ASP:OD2	1:A:77:ALA:HB3	2.02	0.58
5:A:486:HOH:O	2:B:137:LYS:HE3	2.04	0.58
2:B:80:GLN:CD	2:B:80:GLN:H	2.08	0.57
2:D:100:PRO:O	2:D:127:VAL:HB	2.04	0.57
1:A:216:GLU:H	1:A:216:GLU:CD	2.07	0.57
2:D:46:LEU:N	2:D:46:LEU:HD22	2.20	0.57
5:C:507:HOH:O	2:D:130:ARG:HD2	2.03	0.56
2:D:137:LYS:HE2	5:D:190:HOH:O	2.04	0.56
2:B:45:GLY:HA3	2:B:48:LEU:HD11	1.88	0.56
2:B:102:ARG:HD2	5:B:210:HOH:O	2.05	0.55
2:D:85:ARG:HG2	2:D:85:ARG:HH11	1.69	0.55
2:B:111:ASN:O	2:B:117:HIS:HE1	1.88	0.55
2:D:61:ILE:HD13	2:D:61:ILE:N	2.20	0.55
1:C:226:TYR:OH	1:C:266:PRO:HG3	2.07	0.55
1:A:81:LEU:HA	1:A:86:GLU:HB3	1.89	0.54
1:A:40:LYS:O	1:A:41:HIS:HB2	2.07	0.54
2:D:102:ARG:HB2	2:D:125:PHE:O	2.07	0.54
2:B:96:ARG:HG3	2:B:97:PRO:HD2	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:262:LYS:HE2	5:C:428:HOH:O	2.07	0.54
2:B:108:VAL:HG21	2:B:153:ASN:HB3	1.90	0.53
2:D:16:THR:HG22	2:D:64:THR:O	2.08	0.53
1:C:178:LYS:HE3	5:C:470:HOH:O	2.07	0.53
2:D:134:ILE:N	2:D:134:ILE:HD12	2.24	0.53
2:D:12:ILE:HB	5:D:191:HOH:O	2.08	0.53
2:D:67:SER:O	2:D:71:VAL:HG23	2.08	0.53
2:B:91:VAL:O	2:B:91:VAL:HG13	2.08	0.53
1:A:106:HIS:CG	1:A:107:PRO:HD2	2.44	0.53
1:C:151:ARG:NH2	1:C:154:ASN:O	2.42	0.53
2:D:130:ARG:CG	2:D:131:ALA:H	2.21	0.53
2:D:133:ASP:C	2:D:134:ILE:HD12	2.30	0.53
2:B:47:ASN:OD1	2:D:39:ASP:HA	2.09	0.52
2:D:72:ASP:HB3	2:D:100:PRO:HD3	1.89	0.52
2:D:17:VAL:HG22	2:D:60:LYS:HG2	1.91	0.52
2:D:29:LEU:O	2:D:33:PHE:HB2	2.10	0.52
1:C:214:SER:OG	1:C:217:GLU:HB2	2.10	0.51
2:D:134:ILE:H	2:D:147:HIS:HD2	1.59	0.51
1:C:121:ASN:HA	5:C:523:HOH:O	2.10	0.51
1:A:11:SER:HB2	2:B:142:GLU:OE1	2.10	0.51
2:D:119:GLU:HB3	2:D:120:PRO:HD2	1.93	0.51
2:D:141:CYS:SG	2:D:143:LYS:HB2	2.51	0.51
1:A:81:LEU:O	1:A:81:LEU:HD23	2.12	0.50
1:A:214:SER:HB2	1:A:216:GLU:OE1	2.09	0.50
2:B:76:LEU:HD22	2:B:103:ILE:HD13	1.92	0.50
1:C:15:LEU:O	1:C:178:LYS:CE	2.59	0.50
1:A:81:LEU:HD23	1:A:81:LEU:C	2.32	0.50
1:A:291:ASN:ND2	5:A:429:HOH:O	2.44	0.50
2:B:108:VAL:CG2	2:B:153:ASN:HB3	2.40	0.50
2:B:110:PRO:HG2	2:B:145:PHE:CZ	2.46	0.50
2:D:71:VAL:O	2:D:97:PRO:HB3	2.12	0.50
2:B:22:PRO:HB2	2:B:25:ILE:HG13	1.94	0.50
2:B:34:LYS:HD3	2:B:37:GLU:OE2	2.11	0.50
2:B:128:ARG:NH2	2:B:144:GLU:OE2	2.44	0.50
1:A:279:LYS:HD3	5:A:476:HOH:O	2.12	0.50
2:D:58:LEU:HD23	2:D:59:ILE:N	2.26	0.50
2:D:44:ILE:HG22	2:D:46:LEU:HD22	1.95	0.49
1:A:267:LEU:HB3	1:A:268:PRO:HA	1.94	0.49
1:C:37:GLU:HG3	1:C:40:LYS:HD2	1.93	0.49
1:C:183:ARG:HG2	1:C:183:ARG:NH1	2.20	0.49
2:D:69:ASP:O	2:D:73:GLN:N	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:83:VAL:HG23	2:D:95:SER:HB2	1.95	0.49
1:A:101:ALA:HB2	1:A:304:LEU:HD21	1.95	0.49
2:B:76:LEU:HD22	2:B:103:ILE:CD1	2.43	0.49
2:B:81:ALA:O	2:B:96:ARG:HG3	2.12	0.49
1:C:6:GLN:NE2	5:C:519:HOH:O	2.46	0.49
2:B:41:ARG:HD2	2:B:62:GLU:OE1	2.12	0.49
1:C:1:ALA:HA	1:C:306:ARG:O	2.13	0.49
2:D:10:GLU:HB2	2:D:60:LYS:HZ2	1.76	0.49
2:D:143:LYS:HD2	5:D:180:HOH:O	2.12	0.49
2:B:19:ASP:HB3	2:B:82:THR:HG23	1.95	0.48
2:D:66:LEU:HD22	2:D:70:GLN:OE1	2.13	0.48
2:D:12:ILE:HD13	2:D:12:ILE:H	1.78	0.48
1:C:277:VAL:O	1:C:283:ALA:HB2	2.14	0.48
1:A:232:LYS:HE3	5:A:475:HOH:O	2.13	0.47
1:C:301:ALA:HB1	1:C:308:LEU:HD21	1.95	0.47
1:A:55:THR:O	1:A:59:PHE:HB2	2.14	0.47
2:B:27:PHE:CD2	2:D:36:THR:HG21	2.49	0.47
1:A:138:THR:O	1:A:142:LEU:HG	2.15	0.47
1:C:190:ASP:HB3	5:C:502:HOH:O	2.14	0.47
2:B:50:SER:HB2	2:B:56:LYS:HG3	1.97	0.47
1:A:137:GLN:O	1:A:140:LEU:HG	2.15	0.47
1:C:244:LYS:HA	5:C:516:HOH:O	2.15	0.47
1:A:37:GLU:HG3	1:A:40:LYS:HD2	1.97	0.47
1:C:151:ARG:HG3	1:C:155:LEU:HD21	1.96	0.47
2:B:147:HIS:HB3	5:B:204:HOH:O	2.13	0.47
2:B:32:LEU:HG	2:B:106:VAL:CG1	2.45	0.46
2:D:44:ILE:HG22	2:D:46:LEU:CD2	2.45	0.46
1:A:29:LYS:HD2	1:A:309:VAL:HG21	1.98	0.46
1:A:4:LEU:HD12	1:A:302:LEU:HD13	1.97	0.46
2:D:67:SER:HB2	2:D:70:GLN:CB	2.46	0.46
1:A:81:LEU:HG	1:A:86:GLU:O	2.16	0.46
1:A:212:HIS:ND1	1:A:217:GLU:OE2	2.49	0.46
2:B:30:LEU:HD11	2:B:44:ILE:HD13	1.96	0.46
1:C:1:ALA:HB2	1:C:306:ARG:CG	2.45	0.46
1:C:183:ARG:HD3	1:C:185:TYR:OH	2.16	0.46
1:A:114:LEU:CD2	2:B:121:VAL:HG11	2.46	0.46
1:A:280:THR:HB	1:A:281:PRO:HD2	1.98	0.46
1:C:36:PRO:HA	1:C:65:ARG:O	2.15	0.46
1:A:140:LEU:HD12	1:A:140:LEU:C	2.36	0.45
1:A:213:SER:HB2	5:A:474:HOH:O	2.15	0.45
1:C:167:ARG:NE	3:C:332:6PR:HAA2	1.94	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:68:GLU:CD	2:D:68:GLU:H	2.19	0.45
2:D:59:ILE:HG22	2:D:61:ILE:CD1	2.47	0.45
2:D:61:ILE:HB	2:D:64:THR:HB	1.98	0.45
1:C:37:GLU:OE1	1:C:37:GLU:HA	2.17	0.45
2:D:60:LYS:C	2:D:61:ILE:HD13	2.36	0.45
1:A:232:LYS:HE2	5:A:445:HOH:O	2.15	0.45
2:D:78:ALA:HB1	2:D:81:ALA:HB2	1.99	0.45
1:C:31:LYS:HE2	1:C:294:PHE:CE2	2.52	0.45
1:C:54:ARG:NH2	1:C:268:PRO:HG3	2.32	0.45
2:B:141:CYS:O	2:B:142:GLU:HB2	2.16	0.44
1:C:31:LYS:HE3	5:C:436:HOH:O	2.17	0.44
1:C:162:ASP:HB2	1:C:230:VAL:HA	2.00	0.44
2:D:72:ASP:C	2:D:74:LEU:N	2.70	0.44
1:A:174:GLN:O	1:A:178:LYS:HG3	2.16	0.44
2:D:10:GLU:HB2	2:D:60:LYS:HZ3	1.82	0.44
1:C:81:LEU:HA	1:C:86:GLU:H	1.82	0.44
2:D:101:GLU:OE1	2:D:101:GLU:HA	2.18	0.44
2:B:36:THR:HG21	2:D:27:PHE:CG	2.53	0.44
5:C:529:HOH:O	2:D:143:LYS:HE2	2.18	0.44
2:D:68:GLU:N	5:D:167:HOH:O	2.51	0.44
1:C:193:ALA:HB1	5:C:501:HOH:O	2.18	0.43
1:C:134:HIS:N	1:C:135:PRO:HD3	2.33	0.43
2:B:10:GLU:HG3	2:B:60:LYS:NZ	2.33	0.43
1:C:40:LYS:O	1:C:41:HIS:HB2	2.17	0.43
2:B:30:LEU:O	2:B:34:LYS:HA	2.18	0.43
2:D:110:PRO:HG2	2:D:145:PHE:CZ	2.54	0.43
1:C:81:LEU:C	1:C:81:LEU:HD23	2.39	0.43
2:B:46:LEU:HB2	2:D:42:ILE:HB	1.99	0.43
2:D:129:LYS:HG3	5:D:198:HOH:O	2.19	0.43
2:D:82:THR:HG22	2:D:96:ARG:CZ	2.48	0.43
1:C:137:GLN:O	1:C:140:LEU:HG	2.19	0.43
2:D:67:SER:HB2	2:D:70:GLN:HB2	2.01	0.43
2:B:26:GLY:O	2:B:30:LEU:HG	2.19	0.42
1:A:185:TYR:HD2	1:A:212:HIS:NE2	2.16	0.42
2:B:47:ASN:HA	2:B:55:ARG:HD3	2.00	0.42
2:B:48:LEU:O	2:B:55:ARG:HA	2.19	0.42
1:A:165:TYR:CE2	1:A:235:LEU:HD23	2.53	0.42
2:B:17:VAL:CG2	2:B:86:ILE:HD12	2.49	0.42
1:C:237:PRO:C	1:C:239:GLU:H	2.23	0.42
2:B:17:VAL:HG23	2:B:86:ILE:HD12	2.01	0.42
2:B:32:LEU:HG	2:B:106:VAL:HG11	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:132:ASN:ND2	5:C:498:HOH:O	2.52	0.42
1:C:163:LEU:O	1:C:170:HIS:HE1	2.03	0.42
2:B:36:THR:HG23	5:D:200:HOH:O	2.20	0.42
1:C:293:ILE:O	1:C:297:GLN:HG3	2.20	0.42
2:D:62:GLU:O	2:D:63:ASN:HB2	2.18	0.42
2:B:34:LYS:HE2	2:B:34:LYS:HB3	1.86	0.41
1:C:63:MET:SD	1:C:70:VAL:HG22	2.61	0.41
1:A:189:PRO:HB3	1:A:246:GLN:OE1	2.20	0.41
1:A:243:VAL:HG13	1:A:244:LYS:N	2.33	0.41
2:B:117:HIS:HD2	5:B:199:HOH:O	2.03	0.41
2:D:76:LEU:HD11	2:D:103:ILE:HG13	2.02	0.41
2:D:42:ILE:HG22	2:D:44:ILE:HD11	2.02	0.41
1:C:226:TYR:CZ	1:C:266:PRO:HG3	2.56	0.41
2:D:85:ARG:HG2	2:D:85:ARG:NH1	2.35	0.41
1:A:185:TYR:HB3	1:A:212:HIS:HD2	1.86	0.41
2:B:71:VAL:HG13	2:B:83:VAL:HG21	2.03	0.41
2:B:111:ASN:O	2:B:117:HIS:CE1	2.71	0.41
1:C:60:GLU:HG2	1:C:70:VAL:HG11	2.03	0.41
2:D:42:ILE:HG22	2:D:44:ILE:CD1	2.51	0.41
2:D:42:ILE:HG12	2:D:61:ILE:HG23	2.03	0.41
1:C:165:TYR:CE2	1:C:235:LEU:HD23	2.56	0.41
1:C:301:ALA:O	1:C:305:ASN:HB2	2.20	0.41
1:A:205:LYS:HB2	1:A:207:ILE:HG13	2.02	0.40
1:C:17:ARG:NH1	5:C:500:HOH:O	2.53	0.40
1:A:176:LEU:HB3	1:A:184:PHE:HZ	1.86	0.40
2:B:138:CYS:SG	2:B:141:CYS:HB2	2.60	0.40
1:A:192:LEU:HD21	1:A:235:LEU:HD21	2.03	0.40
1:C:163:LEU:HG	1:C:188:ALA:HB2	2.03	0.40
2:D:21:ILE:HB	2:D:57:ASP:HB2	2.01	0.40
1:A:184:PHE:O	1:A:209:TRP:HA	2.22	0.40
2:B:31:SER:HB3	2:D:27:PHE:HZ	1.87	0.40
1:C:24:LEU:HD13	1:C:143:PHE:HA	2.02	0.40
1:C:78:ASN:HB2	5:C:473:HOH:O	2.21	0.40
1:C:106:HIS:CD2	1:C:108:GLN:HB2	2.57	0.40
2:D:44:ILE:HD12	2:D:44:ILE: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)
5:A:489:HOH:O	5:A:489:HOH:O[4_555]	1.57	0.63

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	308/310 (99%)	295 (96%)	11 (4%)	2 (1%)	25	31
1	C	308/310 (99%)	293 (95%)	15 (5%)	0	100	100
2	B	143/153 (94%)	130 (91%)	12 (8%)	1 (1%)	22	26
2	D	143/153 (94%)	127 (89%)	16 (11%)	0	100	100
All	All	902/926 (97%)	845 (94%)	54 (6%)	3 (0%)	41	50

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	131	ALA
1	A	309	VAL
1	A	270	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	261/261 (100%)	252 (97%)	9 (3%)	37	51
1	C	261/261 (100%)	253 (97%)	8 (3%)	40	55
2	B	129/137 (94%)	122 (95%)	7 (5%)	22	30
2	D	129/137 (94%)	124 (96%)	5 (4%)	32	46
All	All	780/796 (98%)	751 (96%)	29 (4%)	34	48

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	LYS
1	A	37	GLU
1	A	59	PHE
1	A	65	ARG
1	A	126	ASN
1	A	134	HIS
1	A	176	LEU
1	A	279	LYS
1	A	285	TYR
2	B	24	GLN
2	B	31	SER
2	B	39	ASP
2	B	56	LYS
2	B	76	LEU
2	B	80	GLN
2	B	141	CYS
1	C	24	LEU
1	C	37	GLU
1	C	59	PHE
1	C	151	ARG
1	C	221	GLU
1	C	261	MET
1	C	285	TYR
1	C	308	LEU
2	D	12	ILE
2	D	37	GLU
2	D	61	ILE
2	D	68	GLU
2	D	94	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	21	ASN
1	A	126	ASN
1	A	132	ASN
1	A	146	GLN
1	A	149	GLN
1	A	174	GLN
1	A	242	ASN
1	A	246	GLN
1	A	260	ASN
1	A	291	ASN

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Mol	Chain	Res	Type
2	B	40	GLN
2	B	47	ASN
2	B	63	ASN
2	B	70	GLN
2	B	73	GLN
2	B	147	HIS
1	C	21	ASN
1	C	33	ASN
1	C	106	HIS
1	C	108	GLN
1	C	132	ASN
1	C	154	ASN
1	C	156	HIS
1	C	170	HIS
1	C	255	HIS
1	C	291	ASN
1	C	297	GLN
1	C	305	ASN
2	D	20	HIS
2	D	40	GLN
2	D	73	GLN
2	D	88	ASN
2	D	147	HIS
2	D	153	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	6PR	A	331	-	15,15,15	1.85	3 (20%)	20,21,21	1.24	2 (10%)
3	6PR	C	332	-	15,15,15	1.83	3 (20%)	20,21,21	1.29	3 (15%)

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	6PR	A	331	-	-	4/17/17/17	-
3	6PR	C	332	-	-	4/17/17/17	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	331	6PR	PAP-OAG	5.35	1.61	1.50
3	C	332	6PR	PAP-OAG	5.31	1.61	1.50
3	A	331	6PR	PAP-OAH	2.88	1.61	1.54
3	C	332	6PR	PAP-OAH	2.84	1.61	1.54
3	A	331	6PR	PAP-OAE	-2.82	1.48	1.54
3	C	332	6PR	PAP-OAE	-2.79	1.48	1.54

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	331	6PR	OAE-PAP-CAJ	3.14	113.44	106.84
3	C	332	6PR	OAE-PAP-CAJ	3.00	113.14	106.84
3	C	332	6PR	OAH-PAP-OAG	-2.43	105.95	112.39
3	A	331	6PR	OAH-PAP-OAG	-2.30	106.31	112.39
3	C	332	6PR	OAG-PAP-CAJ	-2.01	106.35	110.94

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	331	6PR	O-C-CA-N
3	A	331	6PR	NAA-C-CA-N
3	C	332	6PR	O-C-CA-N
3	C	332	6PR	NAA-C-CA-N
3	A	331	6PR	O-C-CA-CB
3	C	332	6PR	O-C-CA-CB
3	A	331	6PR	NAA-C-CA-CB
3	C	332	6PR	NAA-C-CA-CB

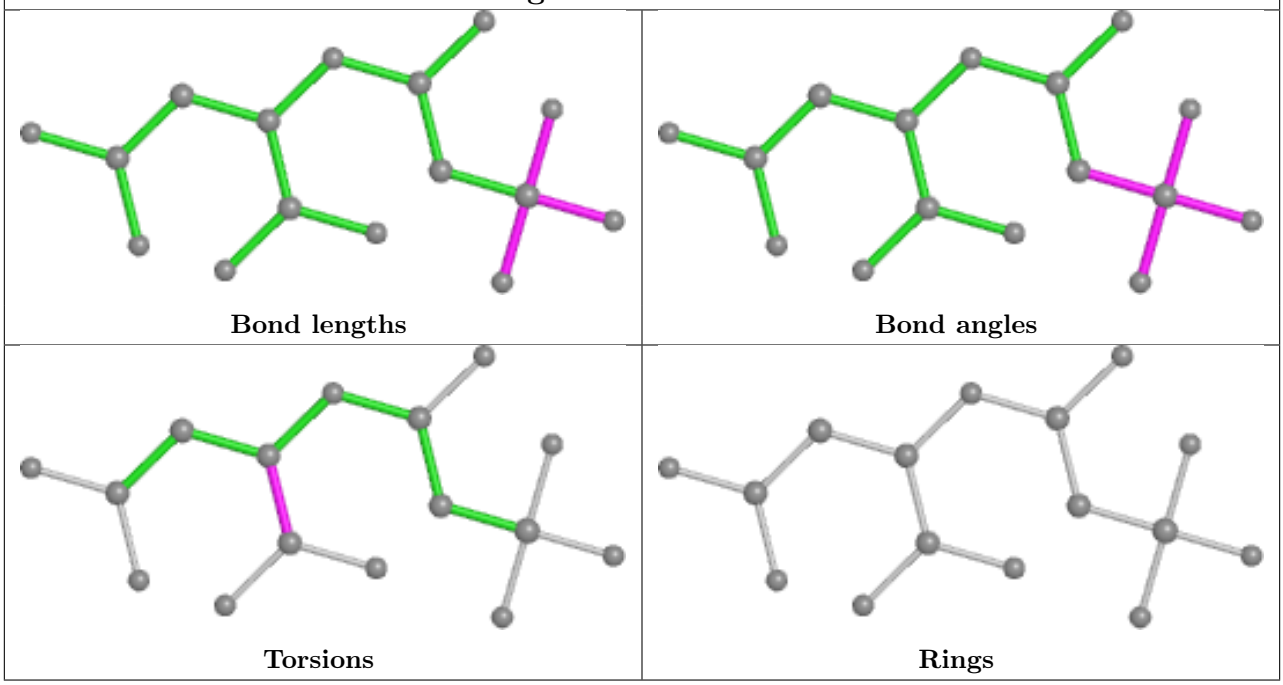
There are no ring outliers.

2 monomers are involved in 5 short contacts:

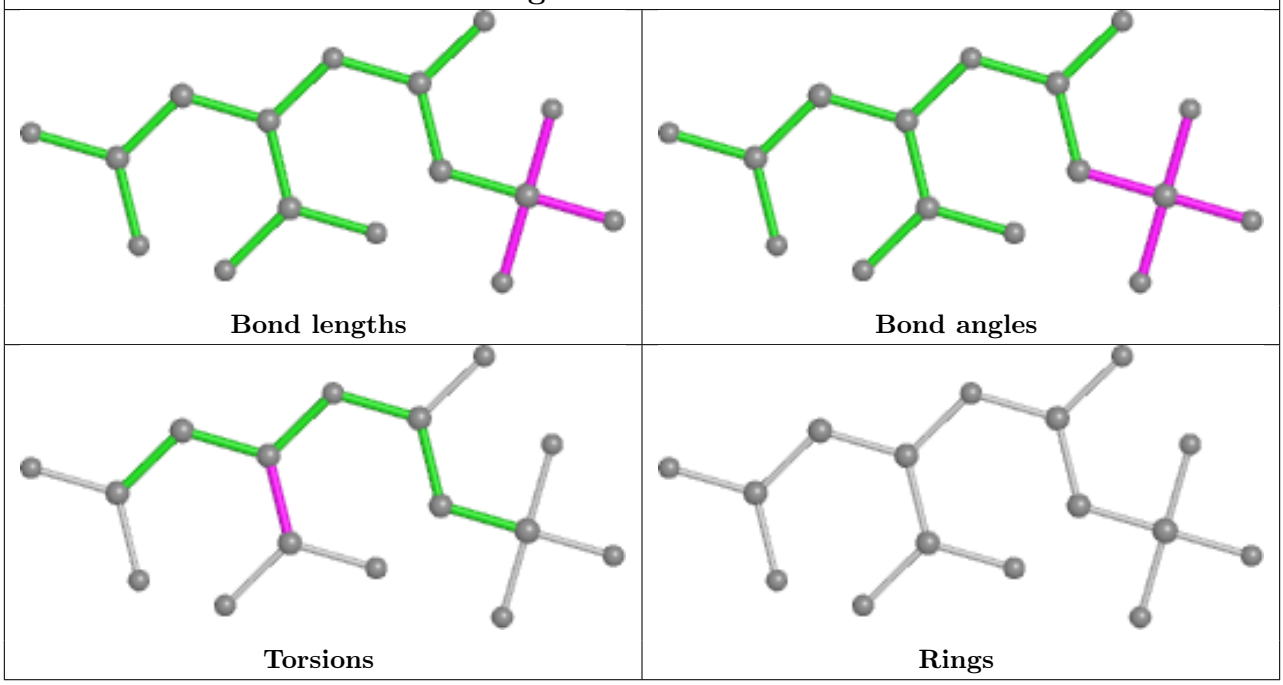
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	331	6PR	3	0
3	C	332	6PR	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand 6PR A 331



Ligand 6PR C 332



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 (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	310/310 (100%)	-0.44	1 (0%) 94 96	21, 35, 53, 99	0
1	C	310/310 (100%)	-0.61	0 100 100	18, 29, 46, 61	0
2	B	145/153 (94%)	0.25	11 (7%) 13 18	30, 53, 84, 114	0
2	D	145/153 (94%)	0.48	13 (8%) 9 12	32, 63, 90, 121	0
All	All	910/926 (98%)	-0.24	25 (2%) 54 62	18, 38, 74, 121	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	9	VAL	14.3
2	D	9	VAL	9.0
2	D	10	GLU	8.2
1	A	310	LEU	8.1
2	D	11	ALA	6.0
2	D	153	ASN	5.9
2	B	10	GLU	5.5
2	B	153	ASN	5.2
2	B	51	GLY	5.1
2	D	89	TYR	3.4
2	D	152	ALA	3.3
2	D	67	SER	3.1
2	D	131	ALA	3.1
2	B	53	MET	3.1
2	B	50	SER	2.9
2	B	52	GLU	2.8
2	D	51	GLY	2.7
2	D	88	ASN	2.7
2	D	52	GLU	2.7
2	D	69	ASP	2.6
2	B	55	ARG	2.5

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Mol	Chain	Res	Type	RSRZ
2	B	49	PRO	2.5
2	B	132	ASN	2.4
2	B	11	ALA	2.3
2	D	13	LYS	2.1

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

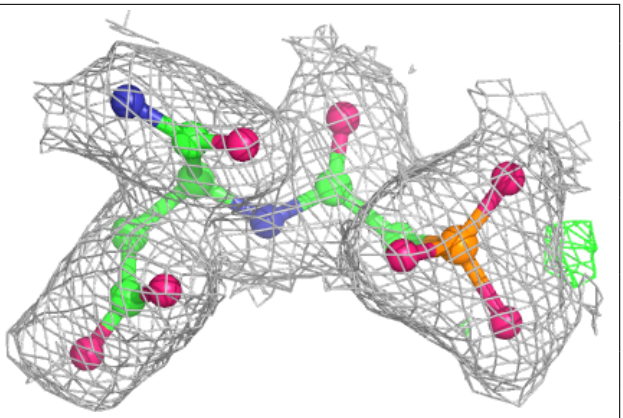
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

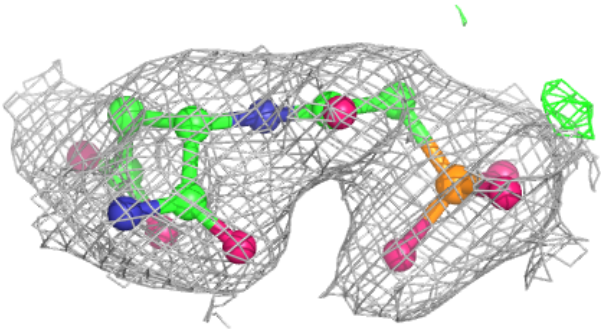
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	6PR	A	331	16/16	0.98	0.14	22,29,31,34	0
3	6PR	C	332	16/16	0.98	0.13	23,26,27,30	0
4	ZN	B	159	1/1	0.99	0.07	38,38,38,38	0
4	ZN	D	159	1/1	1.00	0.04	36,36,36,36	0

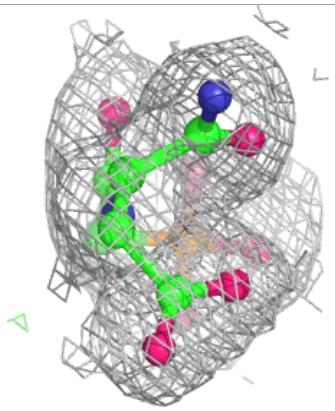
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around 6PR A 331:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

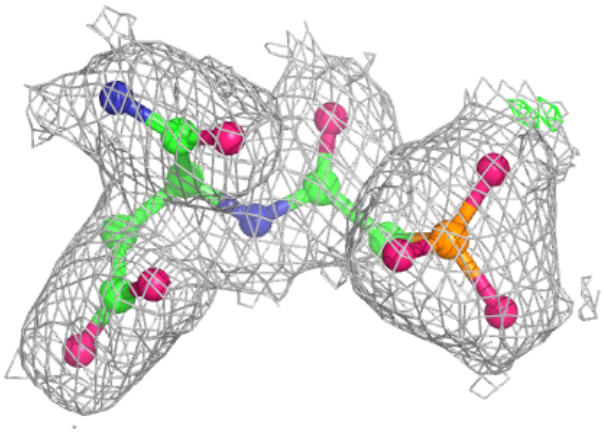


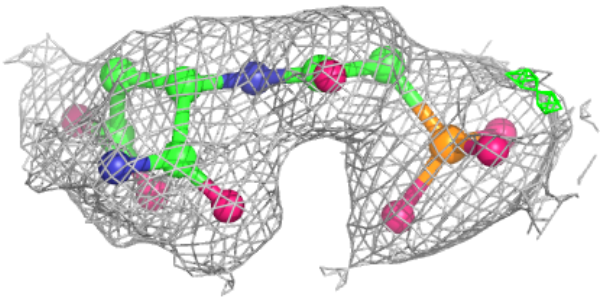


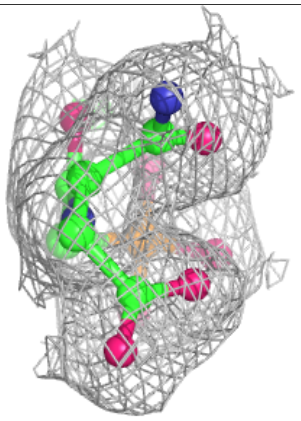


Electron density around 6PR C 332:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)







6.5 Other polymers (i)

There are no such residues in this entry.