



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:10 PM UTC

PDB ID : 1NPY / pdb_00001npy
Title : Structure of shikimate 5-dehydrogenase-like protein HI0607
Authors : Korolev, S.; Koroleva, O.; Zarembinski, T.; Collart, F.; Joachimiak, A.; Midwest Center for Structural Genomics (MCSG)
Deposited on : 2003-01-20
Resolution : 1.75 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

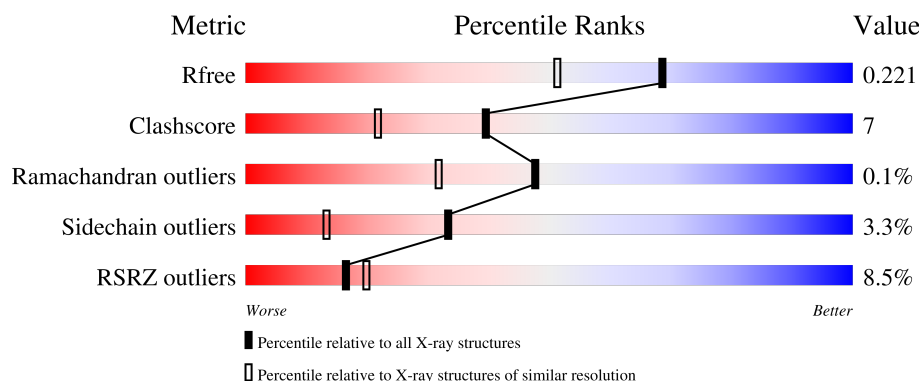
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.75 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}	180053	3183 (1.76-1.76)
Clashscore	190562	3299 (1.76-1.76)
Ramachandran outliers	187476	3274 (1.76-1.76)
Sidechain outliers	187428	3274 (1.76-1.76)
RSRZ outliers	180081	3183 (1.76-1.76)

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 $\leq 5\%$. 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	271	2% 87% 11% ..
1	B	271	3% 88% 11% .
1	C	271	5% 88% 10% .
1	D	271	24% 83% 15% .

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	ACE	D	2002	-	-	X	-

2 Entry composition [i](#)

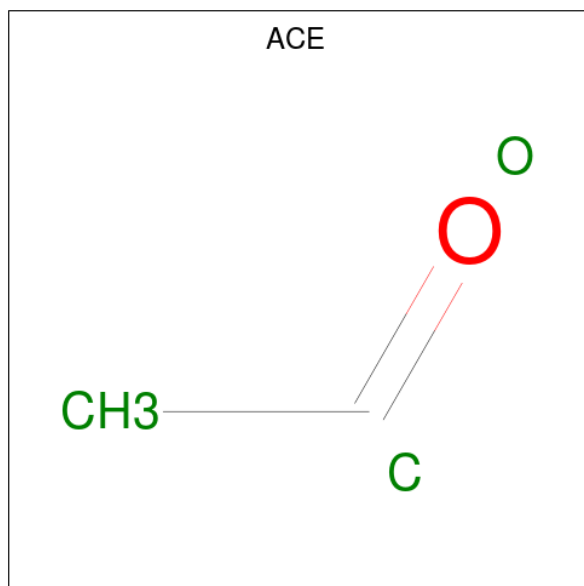
There are 3 unique types of molecules in this entry. The entry contains 9521 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 shikimate 5-dehydrogenase-like protein HI0607.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	269	Total	C	N	O	S	0	0	0
			2087	1337	353	386	11			
1	B	270	Total	C	N	O	S	0	0	0
			2096	1343	355	387	11			
1	C	270	Total	C	N	O	S	0	0	0
			2092	1340	354	387	11			
1	D	270	Total	C	N	O	S	0	0	0
			2088	1338	353	387	10			

- Molecule 2 is ACETYL GROUP (CCD ID: ACE) (formula: C₂H₄O).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	C	O	0	0
			3	2	1		
2	C	1	Total	C	O	0	0
			3	2	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	D	1	Total	C	O	0	0
			3	2	1		

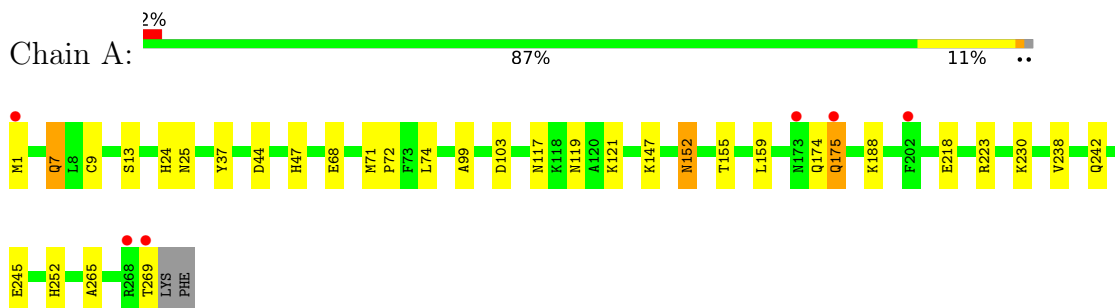
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	332	Total	O	0	0
			332	332		
3	B	325	Total	O	0	0
			325	325		
3	C	300	Total	O	0	0
			300	300		
3	D	192	Total	O	0	0
			192	192		

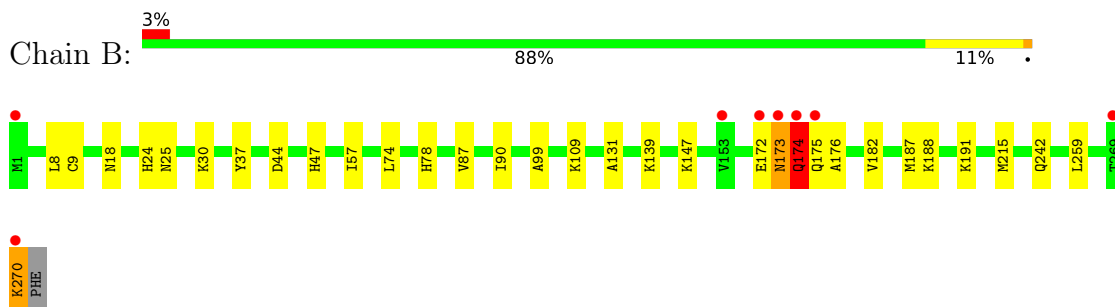
3 Residue-property plots [i](#)

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.

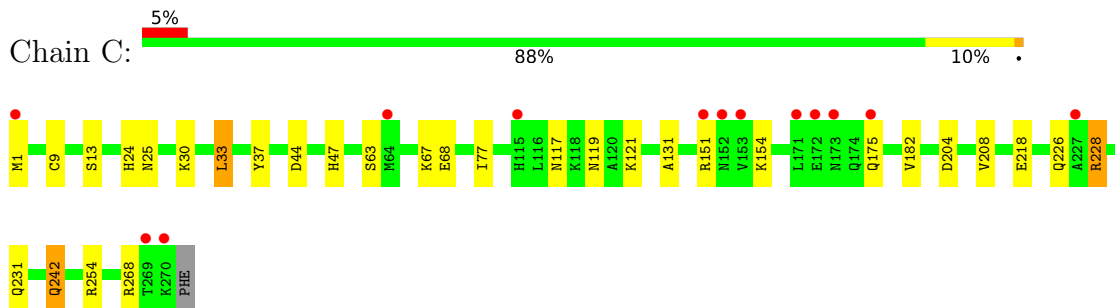
- Molecule 1: Hypothetical shikimate 5-dehydrogenase-like protein HI0607



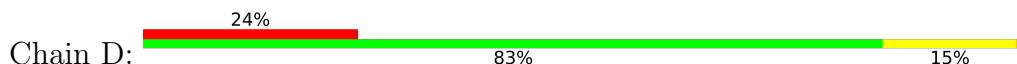
- Molecule 1: Hypothetical shikimate 5-dehydrogenase-like protein HI0607

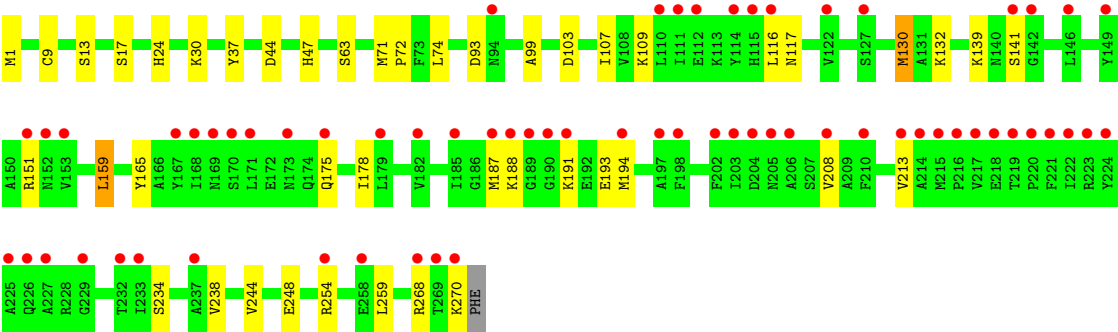


- Molecule 1: Hypothetical shikimate 5-dehydrogenase-like protein HI0607



- Molecule 1: Hypothetical shikimate 5-dehydrogenase-like protein HI0607





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	90.58Å 66.58Å 96.92Å 90.00° 109.56° 90.00°	Depositor
Resolution (Å)	30.00 – 1.75 30.00 – 1.75	Depositor EDS
% Data completeness (in resolution range)	98.4 (30.00-1.75) 98.5 (30.00-1.75)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.91 (at 1.75Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.179 , 0.219 (Not available) , 0.221	Depositor DCC
R_{free} test set	5399 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	14.4	Xtriage
Anisotropy	0.221	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 47.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	9521	wwPDB-VP
Average B, all atoms (Å ²)	19.0	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 34.44 % 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 6.8180e-04. 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, 0.333 respectively for untwinned datasets, and 0.375, 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: ACE

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	0.46	0/2128	1.01	0/2877
1	B	0.49	0/2137	1.04	1/2888 (0.0%)
1	C	0.48	0/2133	1.03	0/2884
1	D	0.42	0/2128	0.99	0/2877
All	All	0.46	0/8526	1.02	1/11526 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	2

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	B	174	GLN	N-CA-C	-5.02	102.64	110.42

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	172	GLU	Peptide
1	B	174	GLN	Peptide

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	2087	0	2095	30	0
1	B	2096	0	2108	26	0
1	C	2092	0	2097	31	0
1	D	2088	0	2096	24	0
2	B	3	0	3	1	0
2	C	3	0	3	1	0
2	D	3	0	3	2	0
3	A	332	0	0	12	0
3	B	325	0	0	9	0
3	C	300	0	0	17	0
3	D	192	0	0	12	0
All	All	9521	0	8405	112	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 7.

All (112) 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:245:GLU:HG3	3:A:569:HOH:O	1.49	1.12
1:D:93:ASP:HB3	3:D:2077:HOH:O	1.56	1.04
1:C:231:GLN:HG2	3:C:2265:HOH:O	1.82	0.78
1:A:7:GLN:HG2	3:A:584:HOH:O	1.83	0.77
1:D:208:VAL:CG2	3:D:2167:HOH:O	2.34	0.75
1:D:244:VAL:O	1:D:248:GLU:HG3	1.88	0.74
1:B:187:MET:HG3	3:B:2247:HOH:O	1.88	0.72
2:D:2002:ACE:H2	3:D:2005:HOH:O	1.88	0.72
1:D:208:VAL:HG21	3:D:2167:HOH:O	1.90	0.71
1:B:18:ASN:HD22	1:B:270:LYS:HD3	1.54	0.71
1:A:25:ASN:HD21	1:A:37:TYR:H	1.36	0.71
1:A:242:GLN:CG	3:A:445:HOH:O	2.38	0.71
1:B:147:LYS:NZ	1:B:174:GLN:OE1	2.21	0.70
1:A:242:GLN:HG3	3:A:445:HOH:O	1.91	0.70
1:B:25:ASN:HD21	1:B:37:TYR:H	1.41	0.69
1:D:130:MET:HE1	1:D:238:VAL:HG11	1.74	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:2003:ACE:HB3	3:C:2052:HOH:O	1.93	0.67
1:C:24:HIS:HD2	3:C:2018:HOH:O	1.76	0.67
1:D:13:SER:HB3	1:D:63:SER:HB2	1.79	0.65
2:B:2001:ACE:H2	3:B:2192:HOH:O	1.96	0.65
1:C:25:ASN:HD21	1:C:37:TYR:H	1.45	0.64
1:B:139:LYS:HE3	3:B:2306:HOH:O	1.97	0.64
1:D:178:ILE:HD11	3:D:2114:HOH:O	1.95	0.64
1:A:121:LYS:NZ	1:A:175:GLN:HG3	2.14	0.63
1:D:47:HIS:HE1	3:D:2073:HOH:O	1.82	0.63
1:B:173:ASN:HB3	1:C:121:LYS:NZ	2.14	0.62
1:B:188:LYS:HD2	1:B:215:MET:HE2	1.81	0.62
1:C:67:LYS:CE	3:C:2288:HOH:O	2.47	0.61
1:A:7:GLN:CG	3:A:584:HOH:O	2.46	0.61
1:A:252:HIS:HE1	3:A:375:HOH:O	1.83	0.61
1:B:8:LEU:HD23	1:B:57:ILE:HD12	1.83	0.61
1:C:131:ALA:HB2	1:C:182:VAL:HG21	1.82	0.60
1:A:147:LYS:NZ	1:A:174:GLN:OE1	2.28	0.60
1:B:18:ASN:ND2	1:B:270:LYS:HD3	2.17	0.60
1:C:121:LYS:HE3	3:C:2254:HOH:O	2.01	0.59
1:B:44:ASP:OD2	1:B:47:HIS:HD2	1.85	0.59
1:A:68:GLU:HG2	3:A:587:HOH:O	2.02	0.59
1:B:191:LYS:HD3	3:B:2305:HOH:O	2.03	0.59
1:A:7:GLN:OE1	3:A:584:HOH:O	2.17	0.57
1:A:103:ASP:OD1	1:A:242:GLN:CD	2.47	0.57
1:C:68:GLU:HG2	3:C:2251:HOH:O	2.06	0.56
1:D:44:ASP:OD2	1:D:47:HIS:HD2	1.89	0.56
1:A:24:HIS:HD2	3:A:286:HOH:O	1.88	0.56
1:B:24:HIS:HD2	3:B:2030:HOH:O	1.89	0.55
1:C:117:ASN:ND2	1:C:119:ASN:H	2.05	0.55
1:C:175:GLN:HB3	3:C:2254:HOH:O	2.06	0.55
1:A:44:ASP:OD2	1:A:47:HIS:HD2	1.90	0.54
1:B:109:LYS:HG2	3:B:2175:HOH:O	2.06	0.54
1:D:30:LYS:HB2	1:D:259:LEU:HD21	1.90	0.54
1:C:44:ASP:OD2	1:C:47:HIS:HD2	1.90	0.54
1:C:13:SER:HB3	1:C:63:SER:HB2	1.89	0.53
1:D:74:LEU:HD13	1:D:99:ALA:HB2	1.89	0.53
1:B:173:ASN:HB3	1:C:121:LYS:HZ3	1.73	0.53
1:C:77:ILE:HD11	3:C:2050:HOH:O	2.07	0.53
1:A:24:HIS:HE1	3:A:332:HOH:O	1.92	0.53
1:B:30:LYS:HG3	1:B:259:LEU:HD11	1.91	0.53
1:C:242:GLN:OE1	3:C:2274:HOH:O	2.19	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:24:HIS:HE1	3:B:2094:HOH:O	1.91	0.53
1:D:193:GLU:HB3	1:D:194:MET:HE2	1.91	0.52
1:B:139:LYS:CE	3:B:2306:HOH:O	2.57	0.51
1:D:24:HIS:HD2	3:D:2024:HOH:O	1.93	0.50
1:A:74:LEU:HD13	1:A:99:ALA:HB2	1.94	0.50
1:A:121:LYS:HZ1	1:A:175:GLN:HG3	1.76	0.50
1:C:67:LYS:NZ	3:C:2288:HOH:O	2.42	0.49
1:C:30:LYS:HE2	3:C:2287:HOH:O	2.12	0.49
1:D:187:MET:HG3	1:D:213:VAL:HG13	1.93	0.49
1:B:74:LEU:HD13	1:B:99:ALA:HB2	1.93	0.49
1:A:218:GLU:OE1	1:A:223:ARG:HG2	2.13	0.49
1:C:131:ALA:CB	1:C:182:VAL:HG21	2.43	0.48
1:C:33:LEU:HD11	3:C:2013:HOH:O	2.13	0.48
1:D:178:ILE:CD1	3:D:2114:HOH:O	2.55	0.48
1:D:93:ASP:OD1	3:D:2052:HOH:O	2.19	0.48
1:B:8:LEU:HD23	1:B:57:ILE:CD1	2.44	0.48
1:A:230:LYS:NZ	3:A:484:HOH:O	2.47	0.47
1:D:103:ASP:O	1:D:107:ILE:HG12	2.14	0.47
1:C:204:ASP:OD1	1:C:228:ARG:CZ	2.63	0.47
1:D:71:MET:N	1:D:72:PRO:CD	2.77	0.47
1:D:139:LYS:HA	1:D:165:TYR:OH	2.14	0.47
1:C:231:GLN:HA	1:C:231:GLN:OE1	2.16	0.46
1:C:254:ARG:HG2	3:C:2232:HOH:O	2.14	0.46
1:A:152:ASN:C	1:A:152:ASN:HD22	2.22	0.46
1:B:215:MET:HE1	3:B:2318:HOH:O	2.15	0.46
1:D:9:CYS:O	1:D:37:TYR:HA	2.15	0.46
1:A:265:ALA:O	1:A:269:THR:HG23	2.16	0.45
1:C:68:GLU:CG	3:C:2251:HOH:O	2.63	0.45
1:C:151:ARG:NE	3:C:2300:HOH:O	2.50	0.44
1:D:116:LEU:HB3	3:D:2114:HOH:O	2.17	0.44
1:D:132:LYS:HG3	1:D:159:LEU:HD21	1.99	0.44
1:A:9:CYS:O	1:A:37:TYR:HA	2.17	0.44
1:D:117:ASN:N	3:D:2114:HOH:O	2.49	0.44
1:A:117:ASN:HD22	1:A:117:ASN:C	2.25	0.44
1:A:223:ARG:HD3	3:A:595:HOH:O	2.17	0.44
1:B:8:LEU:HB3	1:B:57:ILE:HD12	1.99	0.44
1:C:117:ASN:C	1:C:117:ASN:HD22	2.26	0.44
1:C:24:HIS:HE1	3:C:2037:HOH:O	2.00	0.44
1:C:9:CYS:O	1:C:37:TYR:HA	2.17	0.43
1:D:30:LYS:CB	1:D:259:LEU:HD21	2.48	0.43
2:D:2002:ACE:CH3	3:D:2005:HOH:O	2.58	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:152:ASN:ND2	1:A:155:THR:H	2.17	0.42
1:B:175:GLN:CG	1:B:176:ALA:H	2.32	0.42
1:C:13:SER:CB	1:C:63:SER:HB2	2.49	0.42
1:B:9:CYS:O	1:B:37:TYR:HA	2.19	0.42
1:A:117:ASN:ND2	1:A:119:ASN:H	2.17	0.42
1:B:131:ALA:HB2	1:B:182:VAL:HG21	2.01	0.41
1:A:238:VAL:HG12	1:A:242:GLN:OE1	2.20	0.41
1:B:173:ASN:HB3	1:C:121:LYS:HZ1	1.84	0.41
1:B:87:VAL:HG11	1:B:90:ILE:HD11	2.03	0.41
1:A:71:MET:N	1:A:72:PRO:CD	2.83	0.41
1:A:159:LEU:HD23	1:A:159:LEU:HA	1.88	0.41
1:C:154:LYS:NZ	3:C:2262:HOH:O	2.47	0.41
1:A:121:LYS:HE2	1:A:175:GLN:O	2.21	0.40
1:C:218:GLU:OE1	1:C:226:GLN:OE1	2.38	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	267/271 (98%)	265 (99%)	2 (1%)	0	100	100
1	B	268/271 (99%)	265 (99%)	2 (1%)	1 (0%)	30	15
1	C	268/271 (99%)	264 (98%)	4 (2%)	0	100	100
1	D	268/271 (99%)	263 (98%)	5 (2%)	0	100	100
All	All	1071/1084 (99%)	1057 (99%)	13 (1%)	1 (0%)	48	32

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	173	ASN

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	218/220 (99%)	212 (97%)	6 (3%)	38	18
1	B	219/220 (100%)	216 (99%)	3 (1%)	59	44
1	C	218/220 (99%)	212 (97%)	6 (3%)	38	18
1	D	217/220 (99%)	203 (94%)	14 (6%)	15	3
All	All	872/880 (99%)	843 (97%)	29 (3%)	33	13

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

Mol	Chain	Res	Type
1	A	1	MET
1	A	7	GLN
1	A	13	SER
1	A	152	ASN
1	A	175	GLN
1	A	188	LYS
1	B	78	HIS
1	B	242	GLN
1	B	270	LYS
1	C	1	MET
1	C	33	LEU
1	C	208	VAL
1	C	228	ARG
1	C	242	GLN
1	C	268	ARG
1	D	1	MET
1	D	17	SER
1	D	109	LYS
1	D	130	MET
1	D	141	SER
1	D	151	ARG
1	D	159	LEU
1	D	175	GLN
1	D	188	LYS

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Mol	Chain	Res	Type
1	D	191	LYS
1	D	234	SER
1	D	254	ARG
1	D	268	ARG
1	D	270	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	7	GLN
1	A	24	HIS
1	A	25	ASN
1	A	47	HIS
1	A	117	ASN
1	A	152	ASN
1	A	173	ASN
1	A	205	ASN
1	A	252	HIS
1	B	18	ASN
1	B	24	HIS
1	B	25	ASN
1	B	47	HIS
1	B	115	HIS
1	B	119	ASN
1	B	205	ASN
1	C	24	HIS
1	C	25	ASN
1	C	47	HIS
1	C	117	ASN
1	C	119	ASN
1	D	24	HIS
1	D	47	HIS
1	D	174	GLN
1	D	205	ASN
1	D	246	GLN

5.3.3 RNA ⓘ

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

3 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	ACE	D	2002	-	1,2,2	1.60	0	0,1,1	-	-
2	ACE	B	2001	-	1,2,2	1.96	0	0,1,1	-	-
2	ACE	C	2003	-	1,2,2	1.74	0	0,1,1	-	-

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
2	D	2002	ACE	2	0
2	B	2001	ACE	1	0
2	C	2003	ACE	1	0

5.7 Other polymers [i](#)

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, 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	269/271 (99%)	-0.00	6 (2%) 62 69	8, 14, 26, 42	0
1	B	270/271 (99%)	-0.04	8 (2%) 52 59	7, 13, 26, 41	0
1	C	270/271 (99%)	0.21	13 (4%) 35 41	6, 16, 34, 45	0
1	D	270/271 (99%)	1.09	65 (24%) 2 2	9, 24, 46, 57	0
All	All	1079/1084 (99%)	0.31	92 (8%) 16 20	6, 16, 39, 57	0

All (92) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	269	THR	8.4
1	D	227	ALA	6.7
1	D	217	VAL	5.7
1	A	1	MET	4.2
1	D	223	ARG	4.1
1	D	219	THR	4.1
1	D	216	PRO	4.0
1	B	269	THR	4.0
1	B	175	GLN	3.9
1	C	1	MET	3.9
1	B	173	ASN	3.9
1	D	141	SER	3.8
1	D	171	LEU	3.6
1	C	153	VAL	3.6
1	D	149	TYR	3.6
1	A	268	ARG	3.5
1	A	173	ASN	3.5
1	C	175	GLN	3.4
1	D	112	GLU	3.4
1	D	214	ALA	3.3
1	D	198	PHE	3.2

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Mol	Chain	Res	Type	RSRZ
1	D	187	MET	3.2
1	D	111	ILE	3.2
1	D	189	GLY	3.1
1	D	115	HIS	3.1
1	D	190	GLY	3.1
1	C	270	LYS	3.1
1	D	204	ASP	3.0
1	D	153	VAL	3.0
1	B	270	LYS	2.9
1	D	169	ASN	2.9
1	C	173	ASN	2.9
1	D	167	TYR	2.9
1	D	182	VAL	2.8
1	D	122	VAL	2.8
1	D	213	VAL	2.8
1	A	175	GLN	2.8
1	D	110	LEU	2.8
1	D	168	ILE	2.8
1	B	172	GLU	2.7
1	D	142	GLY	2.7
1	D	173	ASN	2.7
1	D	229	GLY	2.7
1	D	202	PHE	2.6
1	C	269	THR	2.6
1	D	208	VAL	2.6
1	D	222	ILE	2.6
1	C	227	ALA	2.6
1	D	170	SER	2.6
1	D	152	ASN	2.6
1	D	185	ILE	2.6
1	D	225	ALA	2.6
1	D	237	ALA	2.6
1	D	175	GLN	2.6
1	C	171	LEU	2.6
1	D	224	TYR	2.6
1	D	194	MET	2.5
1	D	116	LEU	2.5
1	D	226	GLN	2.5
1	D	270	LYS	2.5
1	D	205	ASN	2.5
1	D	210	PHE	2.5
1	D	114	TYR	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	215	MET	2.4
1	C	152	ASN	2.4
1	D	218	GLU	2.4
1	D	197	ALA	2.3
1	A	202	PHE	2.3
1	B	153	VAL	2.3
1	C	151	ARG	2.3
1	D	188	LYS	2.3
1	B	1	MET	2.3
1	C	115	HIS	2.3
1	C	172	GLU	2.2
1	D	268	ARG	2.2
1	D	203	ILE	2.2
1	D	269	THR	2.2
1	D	151	ARG	2.2
1	D	233	ILE	2.2
1	C	64	MET	2.2
1	D	191	LYS	2.2
1	D	146	LEU	2.1
1	D	179	LEU	2.1
1	D	221	PHE	2.1
1	D	254	ARG	2.1
1	D	232	THR	2.1
1	D	206	ALA	2.1
1	B	174	GLN	2.1
1	D	220	PRO	2.1
1	D	258	GLU	2.0
1	D	94	ASN	2.0
1	D	127	SER	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 oligosaccharides 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($\text{\AA}^2$)	Q<0.9
2	ACE	B	2001	3/3	0.57	0.31	13,13,20,21	0
2	ACE	C	2003	3/3	0.64	0.20	23,23,24,25	0
2	ACE	D	2002	3/3	0.83	0.24	15,15,17,21	0

6.5 Other polymers [i](#)

There are no such residues in this entry.