



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 06:09 AM UTC

PDB ID : 1ZCK / pdb_00001zck
Title : native structure prl-1 (ptp4a1)
Authors : Sun, J.P.; Wang, W.Q.; Yang, H.; Liu, S.; Liang, F.; Fedorov, A.A.; Almo, S.C.; Zhang, Z.Y.
Deposited on : 2005-04-12
Resolution : 1.90 Å(reported)

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

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

A user guide is available at

<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

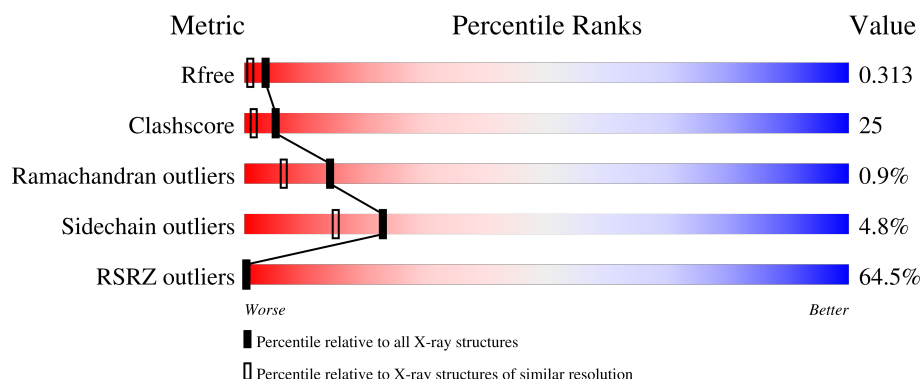
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	154	49% 62% 32% ..
1	B	154	67% 62% 34% ..
1	C	154	71% 58% 37% ...

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	ACY	B	415	-	X	X	-
2	ACY	C	416	-	X	X	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3952 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.

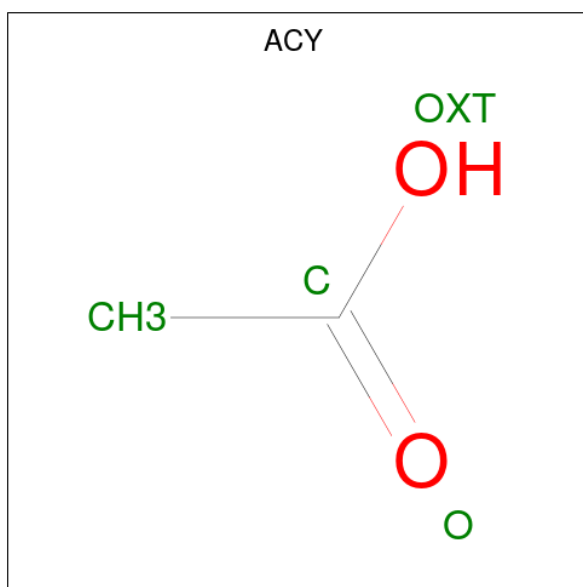
- Molecule 1 is a protein called protein tyrosine phosphatase 4a1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	150	Total	C	N	O	S	Se	0	0	0
			1210	782	210	211	4	3			
1	B	152	Total	C	N	O	S	Se	0	0	0
			1226	790	212	217	4	3			
1	C	152	Total	C	N	O	S	Se	0	0	0
			1226	790	212	217	4	3			

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	17	MSE	MET	modified residue	UNP Q78EG7
A	124	MSE	MET	modified residue	UNP Q78EG7
A	156	MSE	MET	modified residue	UNP Q78EG7
B	17	MSE	MET	modified residue	UNP Q78EG7
B	124	MSE	MET	modified residue	UNP Q78EG7
B	156	MSE	MET	modified residue	UNP Q78EG7
C	17	MSE	MET	modified residue	UNP Q78EG7
C	124	MSE	MET	modified residue	UNP Q78EG7
C	156	MSE	MET	insertion	UNP Q78EG7

- Molecule 2 is ACETIC ACID (CCD ID: ACY) (formula: C₂H₄O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		
2	C	1	Total	C	O	0	0
			4	2	2		

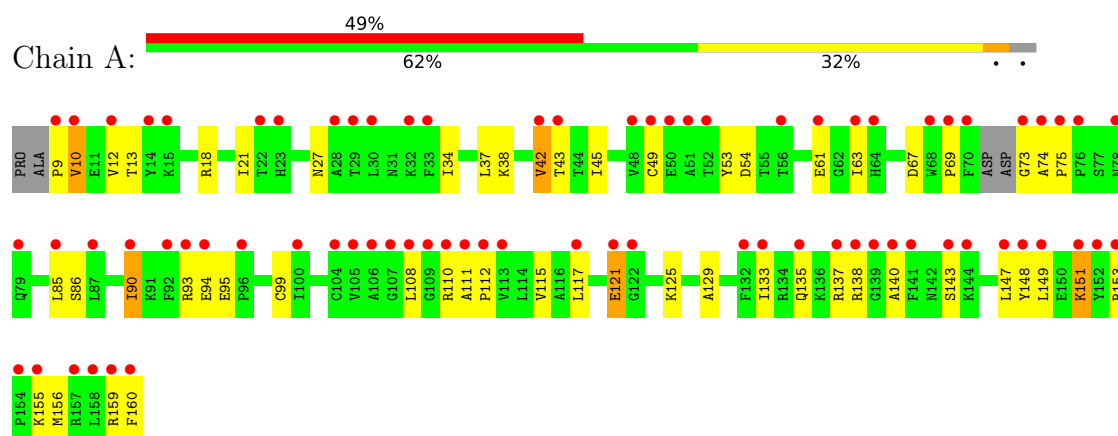
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	82	Total	O	0	0
			82	82		
3	B	99	Total	O	0	0
			99	99		
3	C	97	Total	O	0	0
			97	97		

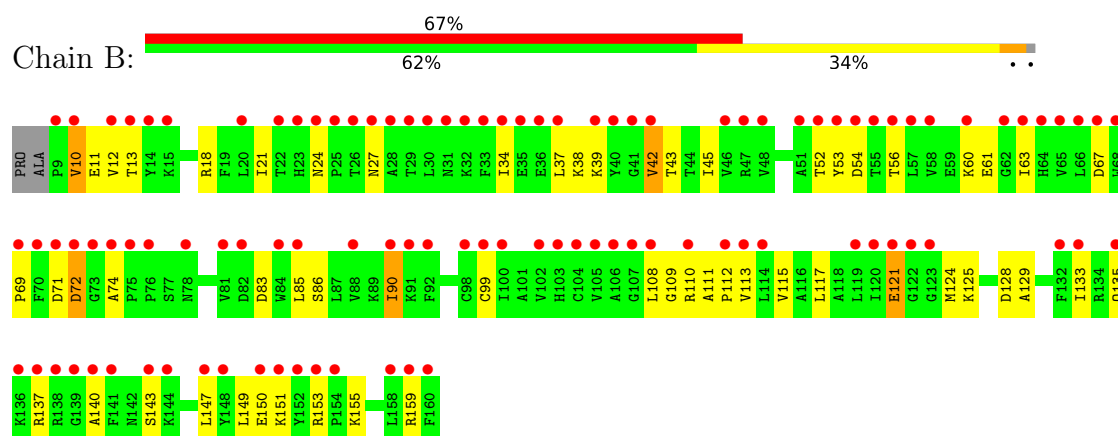
3 Residue-property plots [i](#)

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.

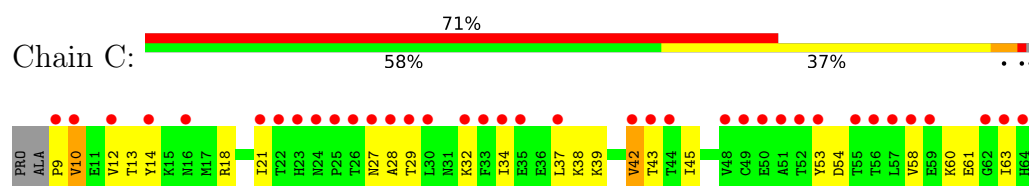
- Molecule 1: protein tyrosine phosphatase 4a1

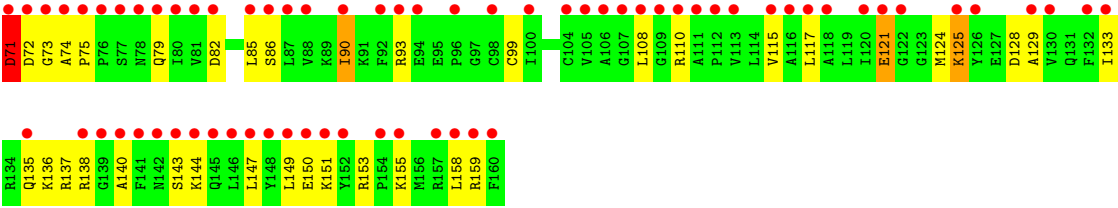


- Molecule 1: protein tyrosine phosphatase 4a1



- Molecule 1: protein tyrosine phosphatase 4a1





4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	71.29Å 105.57Å 181.35Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 1.90 30.00 – 1.92	Depositor EDS
% Data completeness (in resolution range)	(Not available) (30.00-1.90) 92.4 (30.00-1.92)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.91 (at 1.92Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.245 , 0.257 0.307 , 0.313	Depositor DCC
R_{free} test set	4920 reflections (9.48%)	wwPDB-VP
Wilson B-factor (Å ²)	26.8	Xtriage
Anisotropy	0.299	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 37.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	3952	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.07% of the height of the origin peak. No significant pseudotranslation is detected.*

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: ACY

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	0.44	0/1233	0.89	3/1659 (0.2%)
1	B	0.44	0/1250	0.90	4/1684 (0.2%)
1	C	0.46	0/1250	0.89	4/1684 (0.2%)
All	All	0.44	0/3733	0.90	11/5027 (0.2%)

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	125	LYS	N-CA-C	-7.06	101.02	110.55
1	A	125	LYS	N-CA-C	-6.97	101.14	110.55
1	A	90	ILE	N-CA-C	6.87	116.99	110.53
1	B	90	ILE	N-CA-C	6.59	117.38	110.72
1	C	125	LYS	N-CA-C	-6.42	101.01	110.52
1	A	149	LEU	N-CA-C	-5.85	105.03	111.82
1	B	149	LEU	N-CA-C	-5.74	105.16	111.82
1	C	71	ASP	N-CA-C	5.60	122.72	110.80
1	C	149	LEU	N-CA-C	-5.51	105.42	111.82
1	C	90	ILE	N-CA-C	5.45	116.23	110.72
1	B	113	VAL	N-CA-C	5.34	115.55	110.42

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	1210	0	1243	50	2
1	B	1226	0	1252	63	2
1	C	1226	0	1252	81	2
2	A	4	0	3	1	0
2	B	4	0	4	7	0
2	C	4	0	3	3	0
3	A	82	0	0	10	0
3	B	99	0	0	9	1
3	C	97	0	0	28	0
All	All	3952	0	3757	183	4

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 25.

All (183) 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)
2:B:415:ACY:CH3	2:B:415:ACY:C	1.78	1.57
2:B:415:ACY:C	2:B:415:ACY:O	1.67	1.43
1:B:72:ASP:HB3	1:B:110:ARG:NH2	1.74	1.03
1:A:43:THR:HG21	1:A:95:GLU:OE1	1.59	1.01
1:A:155:LYS:HE3	3:A:485:HOH:O	1.65	0.94
1:B:121:GLU:HG3	3:B:476:HOH:O	1.70	0.92
1:B:72:ASP:HB2	3:B:483:HOH:O	1.71	0.89
1:B:150:GLU:HG2	3:B:458:HOH:O	1.77	0.84
1:C:9:PRO:HG2	3:C:466:HOH:O	1.77	0.83
1:C:151:LYS:HD2	3:C:444:HOH:O	1.81	0.80
1:A:121:GLU:HG3	3:A:477:HOH:O	1.81	0.80
1:C:71:ASP:HB2	1:C:74:ALA:HB3	1.64	0.79
1:C:69:PRO:HG3	3:C:500:HOH:O	1.83	0.79
1:C:73:GLY:HA2	3:C:453:HOH:O	1.82	0.78
1:C:10:VAL:HG22	1:C:21:ILE:HB	1.66	0.77
1:C:121:GLU:HG3	3:C:427:HOH:O	1.84	0.77
1:C:158:LEU:HB2	3:C:491:HOH:O	1.83	0.76
1:A:10:VAL:HG22	1:A:21:ILE:HB	1.68	0.75
1:B:10:VAL:HG22	1:B:21:ILE:HB	1.67	0.74
1:C:144:LYS:HE3	3:C:453:HOH:O	1.87	0.74
1:A:73:GLY:HA3	3:A:448:HOH:O	1.87	0.73
1:A:137:ARG:HA	1:A:137:ARG:HE	1.54	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:13:THR:HG22	1:A:18:ARG:HG3	1.70	0.72
1:B:13:THR:HG22	1:B:18:ARG:HG3	1.71	0.71
1:A:9:PRO:HD2	3:A:469:HOH:O	1.88	0.71
1:B:37:LEU:HB3	1:B:42:VAL:CG2	2.20	0.71
1:B:137:ARG:HA	1:B:137:ARG:HE	1.55	0.71
1:A:90:ILE:O	1:A:94:GLU:HG2	1.91	0.70
1:C:137:ARG:HA	1:C:137:ARG:HE	1.56	0.70
1:A:37:LEU:HB3	1:A:42:VAL:CG2	2.21	0.70
1:A:27:ASN:HD21	1:A:54:ASP:H	1.40	0.70
3:A:486:HOH:O	1:C:93:ARG:HG3	1.92	0.69
1:C:13:THR:HG22	1:C:18:ARG:HG3	1.74	0.68
1:C:60:LYS:HD3	1:C:60:LYS:C	2.19	0.68
1:B:37:LEU:HB3	1:B:42:VAL:HG22	1.74	0.68
1:C:37:LEU:HB3	1:C:42:VAL:CG2	2.23	0.68
1:B:71:ASP:O	3:B:507:HOH:O	2.11	0.67
1:C:37:LEU:HB3	1:C:42:VAL:HG22	1.75	0.67
1:A:93:ARG:NH2	3:A:488:HOH:O	2.26	0.67
1:B:27:ASN:HD21	1:B:54:ASP:H	1.41	0.67
1:C:110:ARG:NH2	3:C:445:HOH:O	2.28	0.66
1:C:27:ASN:HD21	1:C:54:ASP:H	1.41	0.66
1:C:73:GLY:CA	3:C:453:HOH:O	2.42	0.66
1:A:37:LEU:HB3	1:A:42:VAL:HG22	1.75	0.66
1:C:12:VAL:HG11	1:C:115:VAL:HG11	1.78	0.65
1:C:73:GLY:N	3:C:445:HOH:O	2.28	0.65
1:B:153:ARG:NH2	3:B:486:HOH:O	2.29	0.65
1:C:34:ILE:HG21	1:C:61:GLU:HG3	1.79	0.64
1:B:72:ASP:C	1:B:74:ALA:H	2.04	0.64
1:C:143:SER:O	1:C:147:LEU:HD23	1.99	0.63
1:C:150:GLU:HG2	3:C:444:HOH:O	1.99	0.63
1:B:34:ILE:HG21	1:B:61:GLU:HG3	1.79	0.63
1:A:12:VAL:HG11	1:A:115:VAL:HG11	1.81	0.63
1:B:143:SER:O	1:B:147:LEU:HD23	1.99	0.63
1:C:29:THR:HA	3:C:424:HOH:O	1.99	0.62
1:C:14:TYR:O	2:C:416:ACY:H2	1.99	0.62
1:C:72:ASP:HA	3:C:445:HOH:O	2.00	0.62
1:A:34:ILE:HG21	1:A:61:GLU:HG3	1.81	0.62
1:A:13:THR:HG22	1:A:18:ARG:CG	2.30	0.61
1:B:12:VAL:HG11	1:B:115:VAL:HG11	1.80	0.61
1:B:13:THR:HG22	1:B:18:ARG:CG	2.29	0.61
2:B:415:ACY:CH3	2:B:415:ACY:O	2.48	0.61
1:A:143:SER:O	1:A:147:LEU:HD23	1.99	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:38:LYS:HE3	1:B:61:GLU:HB3	1.82	0.60
1:C:10:VAL:HG11	1:C:137:ARG:HB2	1.84	0.60
1:B:10:VAL:HA	3:B:469:HOH:O	2.01	0.60
1:A:108:LEU:HD22	1:A:108:LEU:H	1.66	0.60
1:C:29:THR:HG23	3:C:483:HOH:O	2.01	0.59
1:C:13:THR:HG22	1:C:18:ARG:CG	2.31	0.59
1:C:72:ASP:HA	1:C:110:ARG:NH2	2.18	0.59
1:A:135:GLN:HG3	1:C:13:THR:HG23	1.85	0.58
1:B:10:VAL:HG11	1:B:137:ARG:HB2	1.85	0.58
1:C:38:LYS:HE3	1:C:61:GLU:HB3	1.85	0.58
1:C:121:GLU:HG3	3:C:491:HOH:O	2.03	0.58
1:A:135:GLN:HG3	1:C:13:THR:CG2	2.35	0.56
1:A:38:LYS:HE3	1:A:61:GLU:HB3	1.87	0.56
1:B:13:THR:HG23	1:C:135:GLN:HG3	1.88	0.56
1:A:13:THR:HG23	1:B:135:GLN:HG3	1.88	0.55
1:B:72:ASP:HB3	1:B:110:ARG:CZ	2.33	0.55
1:A:129:ALA:O	1:A:133:ILE:HG12	2.07	0.54
1:B:151:LYS:HD3	3:B:443:HOH:O	2.07	0.54
1:B:71:ASP:HB2	1:B:74:ALA:HB3	1.90	0.54
1:A:67:ASP:C	1:A:69:PRO:HD3	2.34	0.53
2:A:414:ACY:H3	3:A:492:HOH:O	2.08	0.52
1:C:14:TYR:O	2:C:416:ACY:CH3	2.57	0.52
1:C:28:ALA:HB3	3:C:483:HOH:O	2.09	0.52
1:C:29:THR:HG22	3:C:424:HOH:O	2.10	0.52
1:B:13:THR:CG2	1:C:135:GLN:HG3	2.40	0.52
1:B:129:ALA:O	1:B:133:ILE:HG12	2.09	0.51
1:A:13:THR:HG23	1:B:135:GLN:CG	2.41	0.51
1:B:110:ARG:NH2	2:B:415:ACY:OXT	2.43	0.51
1:A:108:LEU:HD11	1:A:137:ARG:HD2	1.93	0.51
1:A:42:VAL:HA	1:A:99:CYS:O	2.11	0.50
1:A:42:VAL:O	1:A:63:ILE:HD12	2.12	0.50
1:B:67:ASP:C	1:B:69:PRO:HD3	2.36	0.50
1:B:13:THR:CG2	1:B:18:ARG:HG3	2.41	0.50
1:C:129:ALA:O	1:C:133:ILE:HG12	2.11	0.50
1:A:135:GLN:CG	1:C:13:THR:HG23	2.42	0.49
1:B:13:THR:HG23	1:C:135:GLN:CG	2.42	0.49
1:B:71:ASP:O	1:B:74:ALA:HB3	2.12	0.49
1:C:136:LYS:NZ	3:C:502:HOH:O	2.38	0.49
1:A:13:THR:CG2	1:B:135:GLN:HG3	2.42	0.48
1:C:14:TYR:O	2:C:416:ACY:C	2.60	0.48
1:C:67:ASP:C	1:C:69:PRO:HD3	2.37	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:137:ARG:HA	1:B:137:ARG:NE	2.27	0.48
1:C:138:ARG:HG2	3:C:463:HOH:O	2.12	0.48
1:A:108:LEU:HD21	1:A:137:ARG:HD3	1.95	0.48
1:B:108:LEU:HD22	1:B:108:LEU:H	1.79	0.48
1:C:150:GLU:CG	3:C:444:HOH:O	2.58	0.48
1:B:42:VAL:O	1:B:63:ILE:HD12	2.14	0.48
1:B:111:ALA:N	1:B:112:PRO:CD	2.76	0.48
1:C:108:LEU:HD22	1:C:108:LEU:N	2.28	0.48
1:B:11:GLU:N	3:B:469:HOH:O	2.45	0.47
1:B:37:LEU:HB3	1:B:42:VAL:HG21	1.94	0.47
1:A:156:MSE:HA	3:A:477:HOH:O	2.14	0.47
1:C:27:ASN:ND2	1:C:53:TYR:HB2	2.29	0.47
1:B:37:LEU:CD1	1:B:45:ILE:HD11	2.44	0.47
1:B:72:ASP:HA	3:B:507:HOH:O	2.15	0.47
1:B:109:GLY:HA2	2:B:415:ACY:H2	1.96	0.47
1:A:27:ASN:ND2	1:A:53:TYR:HB2	2.30	0.46
1:B:27:ASN:ND2	1:B:53:TYR:HB2	2.30	0.46
1:B:38:LYS:CE	1:B:61:GLU:HB3	2.46	0.46
1:B:42:VAL:HA	1:B:99:CYS:O	2.16	0.46
1:C:60:LYS:HD3	1:C:60:LYS:O	2.16	0.46
1:A:37:LEU:HB3	1:A:42:VAL:HG21	1.95	0.46
1:C:37:LEU:CD1	1:C:45:ILE:HD11	2.46	0.46
1:C:125:LYS:NZ	3:C:497:HOH:O	2.29	0.46
1:C:42:VAL:HA	1:C:99:CYS:O	2.15	0.46
1:C:42:VAL:O	1:C:63:ILE:HD12	2.16	0.46
1:C:37:LEU:HB3	1:C:42:VAL:HG21	1.99	0.45
1:B:24:ASN:ND2	1:B:52:THR:OG1	2.44	0.45
1:C:124:MSE:HB3	1:C:128:ASP:HB2	1.99	0.45
1:A:49:CYS:SG	1:A:110:ARG:HD2	2.56	0.45
1:C:144:LYS:CE	3:C:453:HOH:O	2.58	0.45
1:B:109:GLY:CA	2:B:415:ACY:O	2.65	0.45
1:B:39:LYS:HB2	1:C:138:ARG:NH2	2.32	0.45
1:A:37:LEU:CD1	1:A:45:ILE:HD11	2.47	0.45
1:B:72:ASP:C	1:B:74:ALA:N	2.71	0.45
1:A:160:PHE:CE2	3:A:471:HOH:O	2.56	0.44
1:A:137:ARG:HA	1:A:137:ARG:NE	2.27	0.44
1:B:43:THR:O	1:B:43:THR:HG22	2.18	0.44
1:B:109:GLY:HA3	2:B:415:ACY:C	2.48	0.44
1:C:108:LEU:H	1:C:108:LEU:CD2	2.30	0.44
1:A:111:ALA:HB3	1:A:112:PRO:HD3	1.99	0.44
1:B:124:MSE:HB3	1:B:128:ASP:HB2	1.98	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:155:LYS:HD2	3:C:509:HOH:O	2.17	0.44
1:C:137:ARG:HA	1:C:137:ARG:NE	2.29	0.44
1:A:138:ARG:NH2	1:C:39:LYS:HB2	2.32	0.43
1:C:38:LYS:CE	1:C:61:GLU:HB3	2.48	0.43
1:C:86:SER:O	1:C:90:ILE:HG22	2.18	0.43
1:A:135:GLN:CG	1:C:13:THR:CG2	2.96	0.43
1:C:29:THR:CA	3:C:424:HOH:O	2.64	0.43
1:B:86:SER:O	1:B:90:ILE:HG22	2.18	0.43
1:A:38:LYS:CE	1:A:61:GLU:HB3	2.49	0.43
1:C:32:LYS:HG3	3:C:494:HOH:O	2.19	0.43
1:B:72:ASP:O	1:B:74:ALA:N	2.50	0.42
1:B:111:ALA:HB3	1:B:112:PRO:HD3	1.99	0.42
1:B:159:ARG:HG2	1:B:159:ARG:HH11	1.85	0.42
1:C:82:ASP:OD1	1:C:155:LYS:HE3	2.19	0.42
1:A:159:ARG:HG2	1:A:159:ARG:HH11	1.84	0.42
1:B:56:THR:O	1:B:60:LYS:HG2	2.19	0.42
1:C:159:ARG:HH11	1:C:159:ARG:HG2	1.84	0.42
1:A:74:ALA:HA	1:A:75:PRO:HD3	1.92	0.42
1:A:151:LYS:HD3	1:A:151:LYS:HA	1.63	0.42
1:C:151:LYS:CD	3:C:444:HOH:O	2.52	0.42
1:A:13:THR:CG2	1:A:18:ARG:HG3	2.43	0.42
1:B:13:THR:OG1	1:C:135:GLN:HG3	2.20	0.41
1:C:58:VAL:HG12	1:C:63:ILE:HB	2.02	0.41
1:A:86:SER:O	1:A:90:ILE:HG22	2.21	0.41
1:C:60:LYS:C	1:C:60:LYS:CD	2.90	0.41
1:C:72:ASP:C	1:C:74:ALA:H	2.29	0.41
1:C:108:LEU:HD22	1:C:108:LEU:H	1.84	0.41
1:A:160:PHE:HE2	3:A:471:HOH:O	2.01	0.41
1:B:13:THR:CG2	1:C:135:GLN:CG	2.98	0.41
1:C:43:THR:HG22	1:C:43:THR:O	2.20	0.41
1:B:108:LEU:HD22	1:B:108:LEU:N	2.36	0.41
1:C:74:ALA:HA	1:C:75:PRO:HD3	1.94	0.40
1:A:159:ARG:HG2	1:A:159:ARG:NH1	2.36	0.40
1:B:37:LEU:HD22	1:B:42:VAL:HG21	2.04	0.40
1:C:28:ALA:C	3:C:424:HOH:O	2.64	0.40
1:C:159:ARG:HG2	1:C:159:ARG:NH1	2.37	0.40
1:A:13:THR:CG2	1:B:135:GLN:CG	2.99	0.40
1:C:121:GLU:CB	3:C:491:HOH:O	2.68	0.40

All (4) 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)
1:B:83:ASP:OD2	1:C:79:GLN:NE2[7_455]	1.85	0.35
1:A:153:ARG:O	1:C:153:ARG:NH2[3_555]	1.92	0.28
1:A:160:PHE:OXT	1:B:159:ARG:NH1[3_555]	2.07	0.13
3:B:428:HOH:O	3:B:430:HOH:O[3_555]	2.17	0.03

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	146/154 (95%)	138 (94%)	7 (5%)	1 (1%)	18	10
1	B	150/154 (97%)	140 (93%)	9 (6%)	1 (1%)	18	10
1	C	150/154 (97%)	139 (93%)	9 (6%)	2 (1%)	9	3
All	All	446/462 (96%)	417 (94%)	25 (6%)	4 (1%)	14	6

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	71	ASP
1	A	140	ALA
1	B	140	ALA
1	C	140	ALA

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.

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	131/131 (100%)	124 (95%)	7 (5%)	20	12
1	B	133/131 (102%)	126 (95%)	7 (5%)	20	12
1	C	133/131 (102%)	128 (96%)	5 (4%)	29	21
All	All	397/393 (101%)	378 (95%)	19 (5%)	23	15

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	VAL
1	A	42	VAL
1	A	85	LEU
1	A	117	LEU
1	A	121	GLU
1	A	148	TYR
1	A	151	LYS
1	B	10	VAL
1	B	42	VAL
1	B	72	ASP
1	B	85	LEU
1	B	117	LEU
1	B	121	GLU
1	B	155	LYS
1	C	10	VAL
1	C	42	VAL
1	C	85	LEU
1	C	117	LEU
1	C	121	GLU

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

Mol	Chain	Res	Type
1	A	27	ASN
1	B	27	ASN
1	C	27	ASN

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	ACY	B	415	-	3,3,3	7.85	3 (100%)	3,3,3	4.91	2 (66%)
2	ACY	C	416	-	3,3,3	0.89	0	3,3,3	4.33	3 (100%)
2	ACY	A	414	-	3,3,3	1.10	0	3,3,3	3.62	2 (66%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	415	ACY	O-C	10.43	1.67	1.22
2	B	415	ACY	CH3-C	7.42	1.78	1.49
2	B	415	ACY	OXT-C	4.59	1.52	1.30

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	415	ACY	O-C-CH3	-7.39	92.23	122.53
2	C	416	ACY	OXT-C-CH3	-5.88	90.42	115.05
2	A	414	ACY	OXT-C-CH3	-4.69	95.41	115.05
2	C	416	ACY	O-C-CH3	4.12	139.42	122.53
2	A	414	ACY	O-C-CH3	4.08	139.25	122.53
2	B	415	ACY	OXT-C-O	3.77	136.03	122.03
2	C	416	ACY	OXT-C-O	2.19	130.16	122.03

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	415	ACY	7	0
2	C	416	ACY	3	0
2	A	414	ACY	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	147/154 (95%)	2.25	75 (51%) 0 0	19, 33, 46, 58	0
1	B	149/154 (96%)	2.57	103 (69%) 0 0	17, 30, 50, 58	0
1	C	149/154 (96%)	2.75	109 (73%) 0 0	18, 31, 50, 66	0
All	All	445/462 (96%)	2.53	287 (64%) 0 0	17, 32, 50, 66	0

All (287) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	108	LEU	6.8
1	A	148	TYR	6.8
1	C	26	THR	6.7
1	C	140	ALA	6.6
1	C	74	ALA	6.4
1	C	28	ALA	6.0
1	B	9	PRO	5.5
1	A	140	ALA	5.5
1	A	90	ILE	5.3
1	C	68	TRP	5.3
1	B	27	ASN	5.2
1	C	141	PHE	5.1
1	B	56	THR	5.0
1	B	73	GLY	5.0
1	C	108	LEU	4.9
1	A	160	PHE	4.9
1	C	148	TYR	4.8
1	A	106	ALA	4.8
1	C	160	PHE	4.7
1	C	27	ASN	4.7
1	C	72	ASP	4.7
1	C	34	ILE	4.7
1	B	140	ALA	4.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	144	LYS	4.5
1	B	60	LYS	4.5
1	C	107	GLY	4.5
1	C	144	LYS	4.5
1	B	57	LEU	4.5
1	B	28	ALA	4.4
1	C	106	ALA	4.4
1	B	158	LEU	4.4
1	B	70	PHE	4.3
1	A	143	SER	4.3
1	C	75	PRO	4.2
1	C	70	PHE	4.2
1	A	12	VAL	4.2
1	A	9	PRO	4.2
1	B	108	LEU	4.2
1	B	153	ARG	4.1
1	C	105	VAL	4.1
1	C	104	CYS	4.1
1	C	30	LEU	4.1
1	B	84	TRP	4.1
1	B	66	LEU	4.0
1	B	46	VAL	4.0
1	C	118	ALA	4.0
1	A	75	PRO	4.0
1	B	105	VAL	4.0
1	A	105	VAL	3.9
1	B	106	ALA	3.9
1	B	135	GLN	3.9
1	B	34	ILE	3.9
1	C	133	ILE	3.9
1	B	159	ARG	3.8
1	B	37	LEU	3.8
1	B	25	PRO	3.8
1	A	28	ALA	3.8
1	B	10	VAL	3.8
1	C	88	VAL	3.8
1	A	107	GLY	3.7
1	A	104	CYS	3.7
1	C	135	GLN	3.7
1	A	56	THR	3.7
1	B	98	CYS	3.7
1	C	58	VAL	3.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	159	ARG	3.7
1	A	63	ILE	3.7
1	C	122	GLY	3.7
1	C	143	SER	3.6
1	B	90	ILE	3.6
1	B	72	ASP	3.6
1	C	69	PRO	3.6
1	C	57	LEU	3.6
1	C	24	ASN	3.6
1	C	14	TYR	3.5
1	B	88	VAL	3.5
1	C	12	VAL	3.5
1	B	141	PHE	3.5
1	B	14	TYR	3.5
1	A	52	THR	3.5
1	C	81	VAL	3.5
1	B	160	PHE	3.5
1	B	148	TYR	3.5
1	C	126	TYR	3.5
1	A	111	ALA	3.5
1	C	139	GLY	3.5
1	A	94	GLU	3.4
1	C	9	PRO	3.4
1	B	69	PRO	3.4
1	C	159	ARG	3.4
1	C	51	ALA	3.4
1	B	92	PHE	3.4
1	A	23	HIS	3.3
1	C	49	CYS	3.3
1	C	53	TYR	3.3
1	C	147	LEU	3.3
1	A	138	ARG	3.3
1	B	74	ALA	3.3
1	B	76	PRO	3.3
1	C	32	LYS	3.2
1	A	147	LEU	3.2
1	B	75	PRO	3.2
1	A	109	GLY	3.2
1	B	107	GLY	3.2
1	C	90	ILE	3.2
1	A	149	LEU	3.2
1	A	74	ALA	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	10	VAL	3.2
1	B	81	VAL	3.2
1	C	158	LEU	3.2
1	B	122	GLY	3.2
1	C	121	GLU	3.2
1	B	42	VAL	3.1
1	B	48	VAL	3.1
1	A	110	ARG	3.1
1	A	70	PHE	3.1
1	C	22	THR	3.1
1	C	77	SER	3.1
1	C	62	GLY	3.1
1	C	155	LYS	3.1
1	B	26	THR	3.1
1	B	139	GLY	3.1
1	C	113	VAL	3.0
1	A	121	GLU	3.0
1	B	22	THR	3.0
1	C	80	ILE	3.0
1	A	14	TYR	3.0
1	C	132	PHE	3.0
1	C	73	GLY	3.0
1	C	125	LYS	3.0
1	B	137	ARG	3.0
1	C	149	LEU	3.0
1	B	113	VAL	3.0
1	A	51	ALA	3.0
1	B	31	ASN	3.0
1	B	52	THR	2.9
1	C	110	ARG	2.9
1	C	85	LEU	2.9
1	B	15	LYS	2.9
1	A	151	LYS	2.9
1	A	137	ARG	2.9
1	A	42	VAL	2.9
1	B	33	PHE	2.9
1	C	86	SER	2.9
1	C	117	LEU	2.9
1	A	73	GLY	2.9
1	A	69	PRO	2.8
1	C	79	GLN	2.8
1	A	132	PHE	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	68	TRP	2.8
1	B	133	ILE	2.8
1	A	157	ARG	2.8
1	B	144	LYS	2.8
1	C	152	TYR	2.8
1	B	121	GLU	2.8
1	B	54	ASP	2.8
1	B	41	GLY	2.8
1	C	93	ARG	2.8
1	A	15	LYS	2.8
1	C	56	THR	2.8
1	B	32	LYS	2.8
1	B	123	GLY	2.8
1	A	30	LEU	2.8
1	C	63	ILE	2.8
1	C	37	LEU	2.7
1	C	154	PRO	2.7
1	A	79	GLN	2.7
1	C	10	VAL	2.7
1	C	98	CYS	2.7
1	C	71	ASP	2.7
1	C	146	LEU	2.7
1	A	64	HIS	2.7
1	B	104	CYS	2.7
1	C	29	THR	2.7
1	C	44	THR	2.7
1	C	150	GLU	2.7
1	B	62	GLY	2.6
1	A	68	TRP	2.6
1	A	49	CYS	2.6
1	C	55	THR	2.6
1	C	94	GLU	2.6
1	B	40	TYR	2.6
1	A	96	PRO	2.6
1	C	76	PRO	2.6
1	A	133	ILE	2.6
1	C	130	VAL	2.6
1	C	92	PHE	2.6
1	A	93	ARG	2.6
1	C	157	ARG	2.6
1	A	135	GLN	2.6
1	C	145	GLN	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	36	GLU	2.6
1	B	63	ILE	2.6
1	C	100	ILE	2.6
1	C	116	ALA	2.6
1	B	143	SER	2.6
1	A	29	THR	2.6
1	B	29	THR	2.6
1	A	154	PRO	2.5
1	A	100	ILE	2.5
1	B	24	ASN	2.5
1	B	78	ASN	2.5
1	C	52	THR	2.5
1	B	138	ARG	2.5
1	C	64	HIS	2.5
1	A	22	THR	2.5
1	A	152	TYR	2.5
1	A	117	LEU	2.5
1	A	122	GLY	2.5
1	B	30	LEU	2.5
1	B	13	THR	2.5
1	B	55	THR	2.5
1	B	99	CYS	2.4
1	C	111	ALA	2.4
1	C	82	ASP	2.4
1	C	142	ASN	2.4
1	B	64	HIS	2.4
1	B	147	LEU	2.4
1	A	141	PHE	2.4
1	B	100	ILE	2.4
1	C	67	ASP	2.4
1	B	51	ALA	2.4
1	A	61	GLU	2.4
1	A	113	VAL	2.4
1	B	67	ASP	2.3
1	A	158	LEU	2.3
1	B	114	LEU	2.3
1	A	78	ASN	2.3
1	C	23	HIS	2.3
1	C	96	PRO	2.3
1	A	32	LYS	2.3
1	A	155	LYS	2.3
1	C	138	ARG	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	85	LEU	2.3
1	C	43	THR	2.3
1	B	23	HIS	2.3
1	B	103	HIS	2.3
1	C	115	VAL	2.3
1	B	35	GLU	2.3
1	B	20	LEU	2.3
1	B	85	LEU	2.3
1	C	129	ALA	2.3
1	B	150	GLU	2.3
1	A	87	LEU	2.3
1	B	53	TYR	2.2
1	B	154	PRO	2.2
1	B	71	ASP	2.2
1	C	120	ILE	2.2
1	B	102	VAL	2.2
1	C	78	ASN	2.2
1	B	136	LYS	2.2
1	C	112	PRO	2.2
1	A	33	PHE	2.2
1	A	92	PHE	2.2
1	C	21	ILE	2.2
1	B	91	LYS	2.2
1	A	153	ARG	2.2
1	B	110	ARG	2.2
1	C	25	PRO	2.2
1	B	152	TYR	2.2
1	C	33	PHE	2.2
1	B	39	LYS	2.2
1	C	35	GLU	2.2
1	C	59	GLU	2.2
1	B	12	VAL	2.2
1	B	119	LEU	2.2
1	A	50	GLU	2.1
1	B	120	ILE	2.1
1	B	82	ASP	2.1
1	C	48	VAL	2.1
1	A	139	GLY	2.1
1	B	58	VAL	2.1
1	C	50	GLU	2.1
1	C	16	ASN	2.1
1	C	87	LEU	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	43	THR	2.1
1	B	151	LYS	2.1
1	A	48	VAL	2.1
1	C	42	VAL	2.1
1	A	76	PRO	2.1
1	B	132	PHE	2.0
1	B	47	ARG	2.0
1	C	151	LYS	2.0
1	C	109	GLY	2.0
1	A	112	PRO	2.0
1	B	112	PRO	2.0
1	B	65	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 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(Å ²)	Q<0.9
2	ACY	B	415	4/4	0.33	0.32	59,61,61,62	0
2	ACY	A	414	4/4	0.45	0.20	54,55,55,56	0
2	ACY	C	416	4/4	0.57	0.22	38,45,46,50	0

6.5 Other polymers [i](#)

There are no such residues in this entry.