



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 03:25 AM UTC

PDB ID : 3EYC / pdb_00003eyc
Title : New crystal structure of human tear lipocalin in complex with 1,4-butanediol in space group P21
Authors : Breustedt, D.A.; Keil, L.; Skerra, A.
Deposited on : 2008-10-20
Resolution : 2.60 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

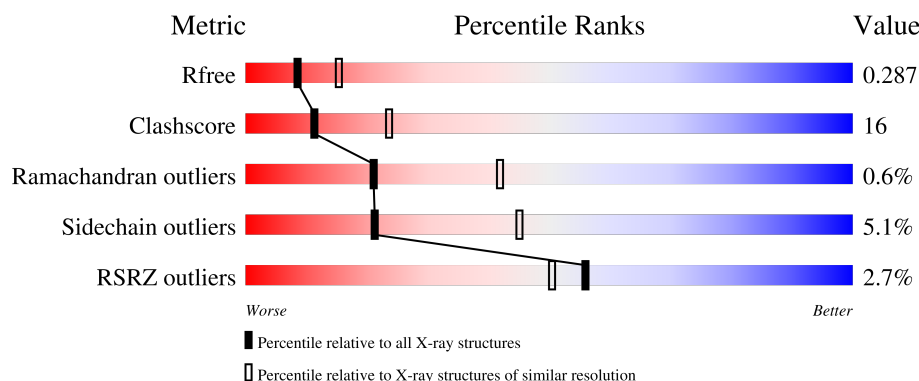
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	162	2% 62% 21% 6% 12%
1	B	162	2% 57% 23% 5% 14%
1	C	162	% 53% 29% 15%
1	D	162	3% 62% 22% 15%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4524 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 Lipocalin-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	143	Total	C	N	O	S	41	0	0
			1106	694	190	216	6			
1	B	140	Total	C	N	O	S	49	0	0
			1090	684	187	213	6			
1	C	137	Total	C	N	O	S	47	0	0
			1058	660	182	210	6			
1	D	137	Total	C	N	O	S	57	0	0
			1061	666	182	208	5			

There are 40 discrepancies between the modelled and reference sequences:

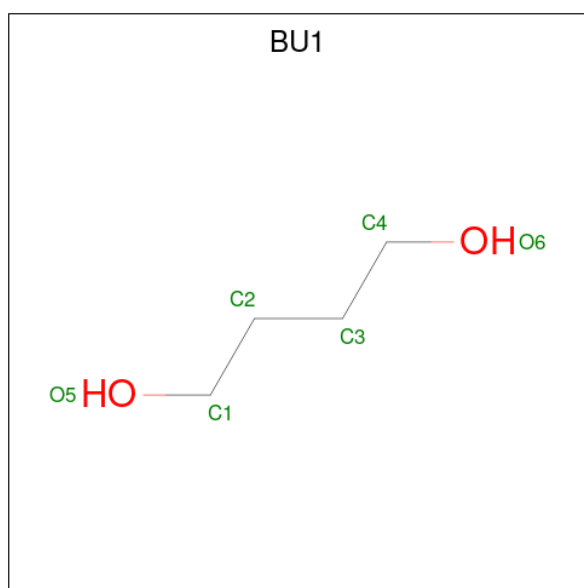
Chain	Residue	Modelled	Actual	Comment	Reference
A	101	SER	CYS	engineered mutation	UNP P31025
A	158	ALA	ASP	engineered mutation	UNP P31025
A	159	TRP	-	expression tag	UNP P31025
A	160	SER	-	expression tag	UNP P31025
A	161	HIS	-	expression tag	UNP P31025
A	162	PRO	-	expression tag	UNP P31025
A	163	GLN	-	expression tag	UNP P31025
A	164	PHE	-	expression tag	UNP P31025
A	165	GLU	-	expression tag	UNP P31025
A	166	LYS	-	expression tag	UNP P31025
B	101	SER	CYS	engineered mutation	UNP P31025
B	158	ALA	ASP	engineered mutation	UNP P31025
B	159	TRP	-	expression tag	UNP P31025
B	160	SER	-	expression tag	UNP P31025
B	161	HIS	-	expression tag	UNP P31025
B	162	PRO	-	expression tag	UNP P31025
B	163	GLN	-	expression tag	UNP P31025
B	164	PHE	-	expression tag	UNP P31025
B	165	GLU	-	expression tag	UNP P31025
B	166	LYS	-	expression tag	UNP P31025
C	101	SER	CYS	engineered mutation	UNP P31025

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	158	ALA	ASP	engineered mutation	UNP P31025
C	159	TRP	-	expression tag	UNP P31025
C	160	SER	-	expression tag	UNP P31025
C	161	HIS	-	expression tag	UNP P31025
C	162	PRO	-	expression tag	UNP P31025
C	163	GLN	-	expression tag	UNP P31025
C	164	PHE	-	expression tag	UNP P31025
C	165	GLU	-	expression tag	UNP P31025
C	166	LYS	-	expression tag	UNP P31025
D	101	SER	CYS	engineered mutation	UNP P31025
D	158	ALA	ASP	engineered mutation	UNP P31025
D	159	TRP	-	expression tag	UNP P31025
D	160	SER	-	expression tag	UNP P31025
D	161	HIS	-	expression tag	UNP P31025
D	162	PRO	-	expression tag	UNP P31025
D	163	GLN	-	expression tag	UNP P31025
D	164	PHE	-	expression tag	UNP P31025
D	165	GLU	-	expression tag	UNP P31025
D	166	LYS	-	expression tag	UNP P31025

- Molecule 2 is 1,4-BUTANEDIOL (CCD ID: BU1) (formula: $C_4H_{10}O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			6	4	2		
2	B	1	Total	C	O	0	0
			6	4	2		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	C	1	Total	C	O	0	0
			6	4	2		
2	D	1	Total	C	O	0	0
			6	4	2		

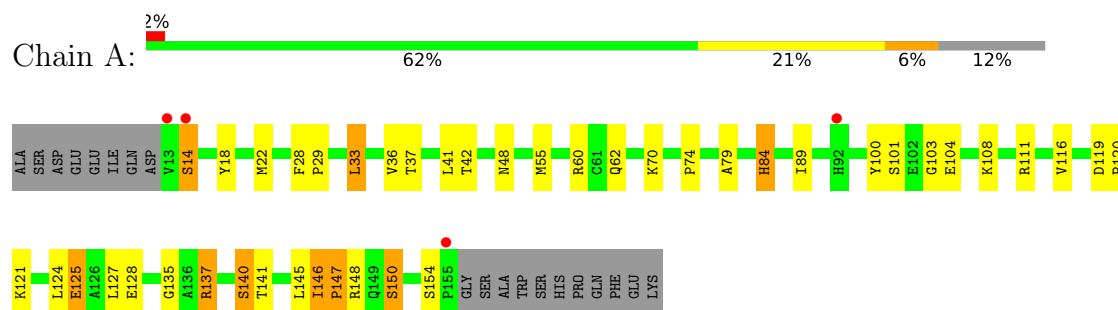
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	42	Total	O	0	0
			42	42		
3	B	34	Total	O	0	0
			34	34		
3	C	55	Total	O	0	0
			55	55		
3	D	54	Total	O	0	0
			54	54		

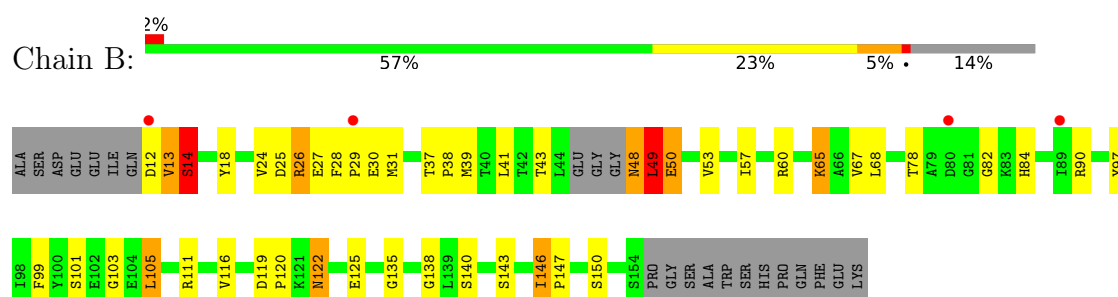
3 Residue-property plots [i](#)

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.

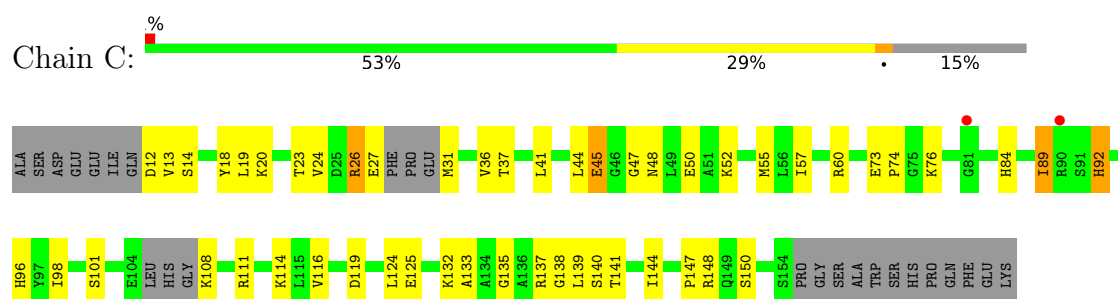
• Molecule 1: Lipocalin-1



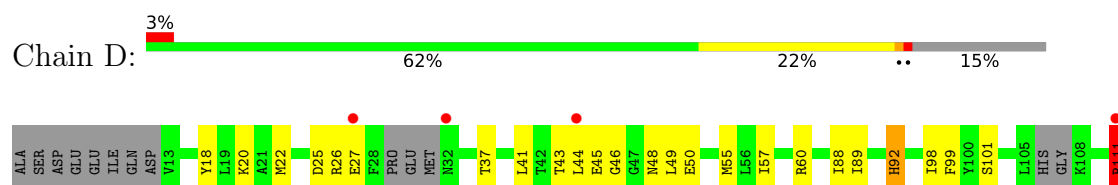
• Molecule 1: Lipocalin-1



• Molecule 1: Lipocalin-1



• Molecule 1: Lipocalin-1





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	63.91Å 34.17Å 143.48Å 90.00° 90.35° 90.00°	Depositor
Resolution (Å)	20.00 – 2.60 20.00 – 2.60	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.00-2.60) 99.4 (20.00-2.60)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.34 (at 2.59Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.228 , 0.274 0.243 , 0.287	Depositor DCC
R_{free} test set	1003 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å ²)	44.8	Xtriage
Anisotropy	0.224	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 55.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.032 for h,-k,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	4524	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.18% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: BU1

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	0.57	1/1126 (0.1%)	1.10	13/1520 (0.9%)
1	B	0.54	0/1108	1.25	17/1494 (1.1%)
1	C	0.54	0/1072	1.06	9/1442 (0.6%)
1	D	0.55	1/1076 (0.1%)	0.99	5/1448 (0.3%)
All	All	0.55	2/4382 (0.0%)	1.11	44/5904 (0.7%)

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	D	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	14	SER	CA-CB	-6.20	1.43	1.53
1	D	22	MET	SD-CE	5.07	1.92	1.79

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	48	ASN	CB-CG-ND2	-11.30	99.45	116.40
1	B	50	GLU	CB-CA-C	-8.90	95.39	110.16
1	A	125	GLU	CB-CA-C	8.89	127.73	110.67
1	B	48	ASN	CB-CG-OD1	8.34	137.48	120.80
1	B	50	GLU	N-CA-CB	8.32	123.63	110.65
1	C	23	THR	CA-C-N	-7.91	110.82	122.68
1	C	23	THR	C-N-CA	-7.91	110.82	122.68

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	108	LYS	CA-C-N	7.40	127.16	119.76
1	C	108	LYS	C-N-CA	7.40	127.16	119.76
1	A	14	SER	N-CA-CB	-7.25	99.32	109.97
1	C	45	GLU	N-CA-C	7.15	118.77	110.97
1	B	49	LEU	N-CA-CB	7.11	124.31	111.37
1	B	48	ASN	CB-CA-C	7.08	123.55	110.10
1	B	50	GLU	CA-CB-CG	7.04	128.17	114.10
1	B	49	LEU	CB-CA-C	-7.00	94.74	109.38
1	A	146	ILE	CA-C-N	6.89	126.92	119.89
1	A	146	ILE	C-N-CA	6.89	126.92	119.89
1	A	125	GLU	CA-CB-CG	6.73	127.57	114.10
1	A	125	GLU	CG-CD-OE1	6.72	133.87	118.40
1	A	125	GLU	CG-CD-OE2	-6.68	103.03	118.40
1	A	125	GLU	CB-CG-CD	6.59	123.80	112.60
1	B	14	SER	CA-CB-OG	6.55	124.21	111.10
1	A	125	GLU	N-CA-CB	-6.42	100.33	110.28
1	B	48	ASN	N-CA-CB	-6.03	100.24	110.50
1	D	147	PRO	N-CA-C	5.96	120.58	111.11
1	C	147	PRO	N-CA-C	5.85	120.42	111.11
1	B	48	ASN	CA-CB-CG	5.77	118.37	112.60
1	A	14	SER	CB-CA-C	-5.56	100.14	109.65
1	B	147	PRO	N-CA-C	5.50	119.86	111.11
1	D	146	ILE	CA-C-N	5.37	125.37	119.89
1	D	146	ILE	C-N-CA	5.37	125.37	119.89
1	C	47	GLY	N-CA-C	-5.19	108.11	115.43
1	B	29	PRO	N-CA-CB	5.19	106.17	102.28
1	A	140	SER	N-CA-C	5.14	118.65	112.38
1	B	26	ARG	CD-NE-CZ	-5.10	117.25	124.40
1	C	60	ARG	CD-NE-CZ	-5.10	117.26	124.40
1	A	147	PRO	N-CA-C	5.07	119.18	111.11
1	B	146	ILE	CA-C-N	5.07	125.06	119.89
1	B	146	ILE	C-N-CA	5.07	125.06	119.89
1	A	60	ARG	CD-NE-CZ	-5.07	117.30	124.40
1	B	60	ARG	CD-NE-CZ	-5.07	117.31	124.40
1	D	26	ARG	CD-NE-CZ	-5.07	117.31	124.40
1	D	60	ARG	CD-NE-CZ	-5.06	117.32	124.40
1	C	26	ARG	CD-NE-CZ	-5.06	117.32	124.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	111	ARG	Sidechain

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	1106	0	1104	31	1
1	B	1090	0	1088	39	0
1	C	1058	0	1056	39	0
1	D	1061	0	1063	29	0
2	A	6	0	10	0	0
2	B	6	0	10	0	0
2	C	6	0	10	2	0
2	D	6	0	10	0	0
3	A	42	0	0	7	0
3	B	34	0	0	3	0
3	C	55	0	0	7	0
3	D	54	0	0	3	0
All	All	4524	0	4351	133	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 (133) 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:125:GLU:HB2	3:A:175:HOH:O	1.51	1.10
1:A:125:GLU:CB	3:A:175:HOH:O	1.99	1.08
1:D:44:LEU:HD12	1:D:44:LEU:O	1.56	1.02
1:B:24:VAL:HG22	1:B:143:SER:HB2	1.50	0.94
1:D:44:LEU:HD23	1:D:50:GLU:HB2	1.55	0.89
1:B:111:ARG:NH2	3:B:187:HOH:O	2.06	0.87
1:A:74:PRO:HD2	3:A:178:HOH:O	1.75	0.85
1:C:12:ASP:O	1:C:12:ASP:OD1	1.95	0.84
1:C:50:GLU:OE1	3:C:180:HOH:O	1.97	0.83
1:D:44:LEU:CD2	1:D:50:GLU:HB2	2.09	0.83
1:A:148:ARG:HG3	1:C:141:THR:O	1.80	0.81

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:44:LEU:O	1:D:44:LEU:CD1	2.28	0.81
1:B:24:VAL:CG2	1:B:143:SER:HB2	2.13	0.77
1:A:28:PHE:HZ	1:A:108:LYS:HB2	1.50	0.76
1:D:25:ASP:OD1	1:D:27:GLU:N	2.19	0.75
1:C:84:HIS:HB2	3:C:197:HOH:O	1.84	0.75
1:D:44:LEU:HD12	1:D:48:ASN:O	1.88	0.72
1:A:119:ASP:OD2	1:A:121:LYS:HB3	1.89	0.72
1:B:48:ASN:N	3:B:172:HOH:O	2.23	0.72
1:B:25:ASP:OD1	1:B:27:GLU:HB2	1.89	0.72
1:C:89:ILE:H	1:C:89:ILE:HD13	1.57	0.69
1:A:125:GLU:HB3	3:A:175:HOH:O	1.73	0.67
1:B:12:ASP:O	1:B:13:VAL:HB	1.95	0.66
1:B:78:THR:OG1	1:B:82:GLY:HA2	1.94	0.66
1:A:28:PHE:CZ	1:A:108:LYS:HB2	2.33	0.64
1:D:44:LEU:HD12	1:D:48:ASN:C	2.24	0.63
1:B:48:ASN:HA	1:B:68:LEU:O	1.99	0.62
1:B:41:LEU:HG	1:B:49:LEU:HD23	1.83	0.61
1:B:84:HIS:ND1	1:B:103:GLY:HA3	2.15	0.61
1:A:100:TYR:CD1	1:A:137:ARG:HG2	2.38	0.59
1:A:89:ILE:HG22	3:A:174:HOH:O	2.04	0.57
1:A:33:LEU:HG	1:A:55:MET:HE2	1.85	0.57
1:A:18:TYR:CE1	1:A:120:PRO:HD3	2.39	0.56
1:D:44:LEU:CD1	1:D:48:ASN:C	2.79	0.56
1:D:43:THR:HA	1:D:49:LEU:HD23	1.87	0.56
1:B:90:ARG:HG3	1:B:97:TYR:CE2	2.41	0.56
1:C:13:VAL:HG12	1:C:41:LEU:HD13	1.88	0.55
1:D:154:SER:N	3:D:193:HOH:O	2.37	0.55
1:B:25:ASP:OD1	1:B:27:GLU:CB	2.55	0.55
1:C:31:MET:HG3	1:C:57:ILE:CG2	2.36	0.55
1:B:28:PHE:CZ	1:B:105:LEU:HB3	2.40	0.55
1:C:89:ILE:HD13	1:C:89:ILE:N	2.22	0.55
1:D:55:MET:HE2	1:D:57:ILE:HD11	1.87	0.54
1:D:18:TYR:CE1	1:D:120:PRO:HD3	2.43	0.54
1:A:84:HIS:CD2	1:A:103:GLY:HA3	2.43	0.54
1:A:62:GLN:HE21	1:A:62:GLN:HA	1.73	0.53
1:B:18:TYR:O	1:B:116:VAL:HA	2.09	0.53
1:B:41:LEU:HD12	1:B:50:GLU:O	2.08	0.53
1:C:41:LEU:HD11	2:C:1:BU1:O5	2.09	0.53
1:B:26:ARG:C	1:B:28:PHE:H	2.14	0.52
1:D:18:TYR:O	1:D:116:VAL:HA	2.09	0.52
1:D:119:ASP:OD1	1:D:120:PRO:HD2	2.09	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:19:LEU:HD11	1:C:114:LYS:HB3	1.91	0.51
1:A:18:TYR:O	1:A:116:VAL:HA	2.10	0.51
1:B:12:ASP:C	1:B:14:SER:H	2.19	0.51
1:B:28:PHE:HZ	1:B:105:LEU:HB3	1.76	0.51
1:C:139:LEU:HA	3:C:188:HOH:O	2.11	0.51
1:C:31:MET:HG3	1:C:57:ILE:HG21	1.94	0.50
1:A:79:ALA:HA	3:A:182:HOH:O	2.11	0.50
1:A:128:GLU:HB2	1:C:124:LEU:HD13	1.93	0.50
1:C:36:VAL:HG23	1:C:55:MET:HG2	1.93	0.50
1:C:26:ARG:O	1:C:27:GLU:HB2	2.11	0.50
1:A:100:TYR:CE1	1:A:137:ARG:HG2	2.47	0.50
1:B:18:TYR:CE1	1:B:120:PRO:HD3	2.47	0.49
1:D:20:LYS:NZ	1:D:121:LYS:O	2.36	0.49
1:B:67:VAL:O	1:B:67:VAL:HG13	2.12	0.49
1:C:18:TYR:O	1:C:116:VAL:HA	2.11	0.49
1:D:44:LEU:O	1:D:45:GLU:HB2	2.13	0.49
1:D:20:LYS:HD3	1:D:119:ASP:O	2.12	0.49
1:B:41:LEU:HG	1:B:49:LEU:CD2	2.42	0.49
1:A:111:ARG:NH2	1:A:137:ARG:O	2.44	0.49
1:A:135:GLY:HA2	1:A:140:SER:HB3	1.95	0.48
1:C:92:HIS:CD2	1:C:92:HIS:O	2.65	0.48
1:C:20:LYS:HD3	1:C:119:ASP:O	2.14	0.48
1:A:124:LEU:HD23	3:A:188:HOH:O	2.12	0.48
1:B:99:PHE:CD2	1:B:99:PHE:C	2.91	0.48
1:D:153:CYS:HA	3:D:193:HOH:O	2.13	0.48
1:D:44:LEU:CD1	1:D:48:ASN:HB3	2.44	0.47
1:A:141:THR:O	1:C:148:ARG:HG3	2.14	0.47
1:C:20:LYS:NZ	1:C:96:HIS:HE1	2.12	0.47
1:D:37:THR:HA	1:D:150:SER:O	2.14	0.47
1:B:84:HIS:CE1	1:B:103:GLY:HA3	2.50	0.47
1:C:37:THR:HA	1:C:150:SER:O	2.15	0.47
1:C:111:ARG:CD	3:C:203:HOH:O	2.62	0.47
1:A:145:LEU:O	1:A:147:PRO:HD3	2.15	0.47
1:B:37:THR:HA	1:B:150:SER:O	2.14	0.46
1:A:128:GLU:HB2	1:C:124:LEU:CD1	2.45	0.46
1:C:135:GLY:HA2	1:C:140:SER:HB3	1.96	0.46
1:D:44:LEU:HD21	1:D:50:GLU:HB2	1.95	0.46
1:B:26:ARG:C	1:B:28:PHE:N	2.72	0.46
1:B:12:ASP:C	1:B:14:SER:N	2.73	0.46
1:C:20:LYS:CE	1:C:96:HIS:HE1	2.28	0.46
1:A:37:THR:HA	1:A:150:SER:O	2.16	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:48:ASN:ND2	1:A:70:LYS:H	2.15	0.45
1:D:135:GLY:HA2	1:D:140:SER:HB3	1.98	0.45
1:B:125:GLU:HA	1:B:125:GLU:OE1	2.18	0.44
1:D:88:ILE:HG12	1:D:99:PHE:HD1	1.82	0.44
1:B:101:SER:O	1:B:111:ARG:HA	2.17	0.44
1:B:138:GLY:HA2	3:B:189:HOH:O	2.16	0.44
1:B:37:THR:HB	1:B:38:PRO:HD2	1.99	0.44
1:C:138:GLY:O	3:C:188:HOH:O	2.20	0.44
1:B:65:LYS:CB	1:B:65:LYS:NZ	2.81	0.44
1:D:101:SER:O	1:D:111:ARG:HA	2.18	0.44
1:A:22:MET:SD	1:A:33:LEU:HD12	2.58	0.44
1:D:44:LEU:CD1	1:D:48:ASN:CB	2.95	0.44
1:D:89:ILE:HG12	1:D:98:ILE:HB	2.01	0.43
1:D:122:ASN:OD1	3:D:206:HOH:O	2.21	0.43
1:C:140:SER:HB2	3:C:211:HOH:O	2.18	0.43
1:B:65:LYS:HB3	1:B:65:LYS:HZ3	1.84	0.43
1:C:41:LEU:HD11	2:C:1:BU1:H22	2.00	0.43
1:A:28:PHE:N	1:A:29:PRO:HD3	2.34	0.43
1:B:25:ASP:OD1	1:B:27:GLU:N	2.51	0.43
1:A:101:SER:O	1:A:111:ARG:HA	2.19	0.43
1:B:39:MET:HE2	1:B:53:VAL:HG11	2.01	0.42
1:B:119:ASP:OD1	1:B:120:PRO:HD2	2.18	0.42
1:C:44:LEU:HB2	1:C:48:ASN:HB2	2.01	0.42
1:A:36:VAL:HG23	1:A:55:MET:HG2	2.01	0.42
1:B:78:THR:HG1	1:B:82:GLY:HA2	1.82	0.42
1:C:101:SER:O	1:C:111:ARG:HA	2.19	0.42
1:C:18:TYR:HA	3:C:168:HOH:O	2.19	0.42
1:C:20:LYS:NZ	1:C:119:ASP:O	2.53	0.42
1:D:45:GLU:HB3	1:D:46:GLY:H	1.74	0.42
1:A:146:ILE:HB	1:C:144:ILE:HB	2.03	0.41
1:B:31:MET:HB3	1:B:57:ILE:HG21	2.03	0.41
1:B:135:GLY:HA2	1:B:140:SER:HB3	2.02	0.41
1:C:12:ASP:O	1:C:12:ASP:CG	2.60	0.41
1:C:89:ILE:HD13	1:C:98:ILE:O	2.21	0.41
1:D:92:HIS:ND1	1:D:92:HIS:C	2.78	0.41
1:C:73:GLU:OE2	1:C:76:LYS:HD2	2.20	0.40
1:B:122:ASN:HD21	1:B:146:ILE:HD13	1.87	0.40
1:C:20:LYS:HZ1	1:C:96:HIS:HE1	1.67	0.40
1:C:73:GLU:HA	1:C:74:PRO:HD3	1.94	0.40
1:C:133:ALA:O	1:C:137:ARG:HG2	2.22	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the sym-

metry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:104:GLU:OE2	1:A:154:SER:OG[1_545]	2.19	0.01

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	141/162 (87%)	140 (99%)	1 (1%)	0	100	100
1	B	136/162 (84%)	132 (97%)	2 (2%)	2 (2%)	8	18
1	C	131/162 (81%)	128 (98%)	2 (2%)	1 (1%)	16	34
1	D	131/162 (81%)	128 (98%)	3 (2%)	0	100	100
All	All	539/648 (83%)	528 (98%)	8 (2%)	3 (1%)	21	42

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	13	VAL
1	B	30	GLU
1	C	14	SER

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	121/137 (88%)	113 (93%)	8 (7%)	15	34

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	120/137 (88%)	114 (95%)	6 (5%)	22	46
1	C	116/137 (85%)	109 (94%)	7 (6%)	17	37
1	D	116/137 (85%)	113 (97%)	3 (3%)	40	68
All	All	473/548 (86%)	449 (95%)	24 (5%)	21	45

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

Mol	Chain	Res	Type
1	A	14	SER
1	A	33	LEU
1	A	41	LEU
1	A	42	THR
1	A	84	HIS
1	A	127	LEU
1	A	137	ARG
1	A	150	SER
1	B	14	SER
1	B	43	THR
1	B	49	LEU
1	B	65	LYS
1	B	105	LEU
1	B	122	ASN
1	C	24	VAL
1	C	45	GLU
1	C	52	LYS
1	C	89	ILE
1	C	92	HIS
1	C	125	GLU
1	C	132	LYS
1	D	41	LEU
1	D	92	HIS
1	D	111	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	48	ASN
1	A	62	GLN
1	A	84	HIS
1	A	149	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	149	GLN
1	C	48	ASN
1	C	84	HIS
1	C	92	HIS
1	C	96	HIS
1	C	149	GLN
1	D	62	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 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	BU1	D	1	-	5,5,5	0.34	0	4,4,4	0.56	0
2	BU1	A	1	-	5,5,5	0.34	0	4,4,4	0.56	0
2	BU1	C	1	-	5,5,5	0.34	0	4,4,4	0.56	0
2	BU1	B	1	-	5,5,5	0.33	0	4,4,4	0.55	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
2	BU1	D	1	-	-	0/3/3/3	-
2	BU1	A	1	-	-	0/3/3/3	-
2	BU1	C	1	-	-	0/3/3/3	-
2	BU1	B	1	-	-	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.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1	BU1	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 [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	143/162 (88%)	-0.10	4 (2%)	55	49	15, 37, 64, 89	11 (7%)
1	B	140/162 (86%)	0.11	4 (2%)	53	48	18, 45, 75, 145	13 (9%)
1	C	137/162 (84%)	-0.03	2 (1%)	72	68	17, 39, 72, 86	11 (8%)
1	D	137/162 (84%)	0.00	5 (3%)	46	40	21, 38, 66, 93	13 (9%)
All	All	557/648 (85%)	-0.01	15 (2%)	56	50	15, 40, 72, 145	48 (8%)

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	29	PRO	4.7
1	C	81	GLY	4.1
1	D	44	LEU	3.4
1	D	27	GLU	3.3
1	A	92	HIS	3.1
1	D	32	ASN	3.0
1	A	14	SER	2.8
1	B	80	ASP	2.7
1	B	12	ASP	2.7
1	D	154	SER	2.5
1	A	155	PRO	2.4
1	A	13	VAL	2.4
1	D	111	ARG	2.3
1	C	90	ARG	2.3
1	B	89	ILE	2.2

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	BU1	C	1	6/6	0.88	0.12	40,40,41,43	0
2	BU1	B	1	6/6	0.89	0.12	56,57,58,58	0
2	BU1	A	1	6/6	0.90	0.10	34,36,38,40	0
2	BU1	D	1	6/6	0.90	0.12	48,49,50,51	0

6.5 Other polymers [i](#)

There are no such residues in this entry.