



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 02:34 PM UTC

PDB ID : 4NO0 / pdb_00004no0
Title : Crystal structure of non-phosphorylated form of RQA_V phosphopeptide bound to HLA-A2 in complex with LILRB1
Authors : Mohammed, F.; Stones, D.H.; Willcox, B.E.
Deposited on : 2013-11-19
Resolution : 2.70 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

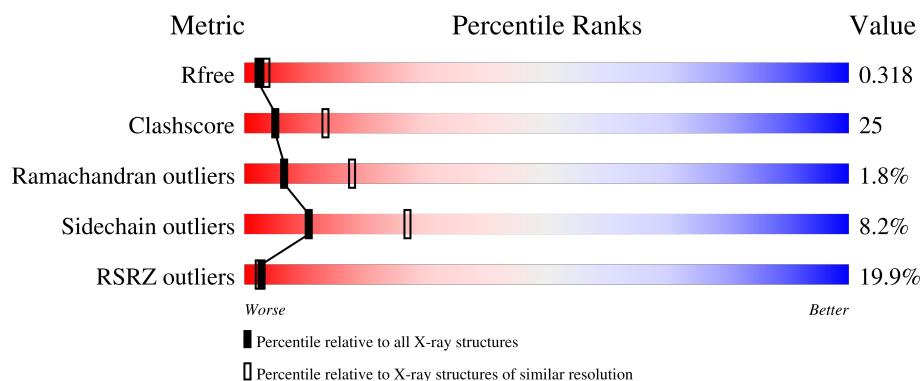
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	276	20% 55% 39% 6%
2	B	99	17% 55% 41% .
3	C	12	58% 25% 50% 25%
4	D	195	18% 57% 36% ...

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 4732 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 HLA class I histocompatibility antigen, A-2 alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	276	Total	C	N	O	S	61	0	0
			2254	1408	410	427	9			

- Molecule 2 is a protein called Beta-2-microglobulin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	99	Total	C	N	O	S	25	0	0
			829	528	140	158	3			

- Molecule 3 is a protein called Lymphocyte-specific protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	12	Total	C	N	O	S	0	0	0
			90	55	16	18	1			

- Molecule 4 is a protein called Leukocyte immunoglobulin-like receptor subfamily B member 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	192	Total	C	N	O	S	36	0	0
			1507	954	261	286	6			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	45	PRO	LEU	SEE REMARK 999	UNP Q8NHL6
D	119	THR	ILE	SEE REMARK 999	UNP Q8NHL6
D	132	ILE	SER	SEE REMARK 999	UNP Q8NHL6

- Molecule 5 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



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

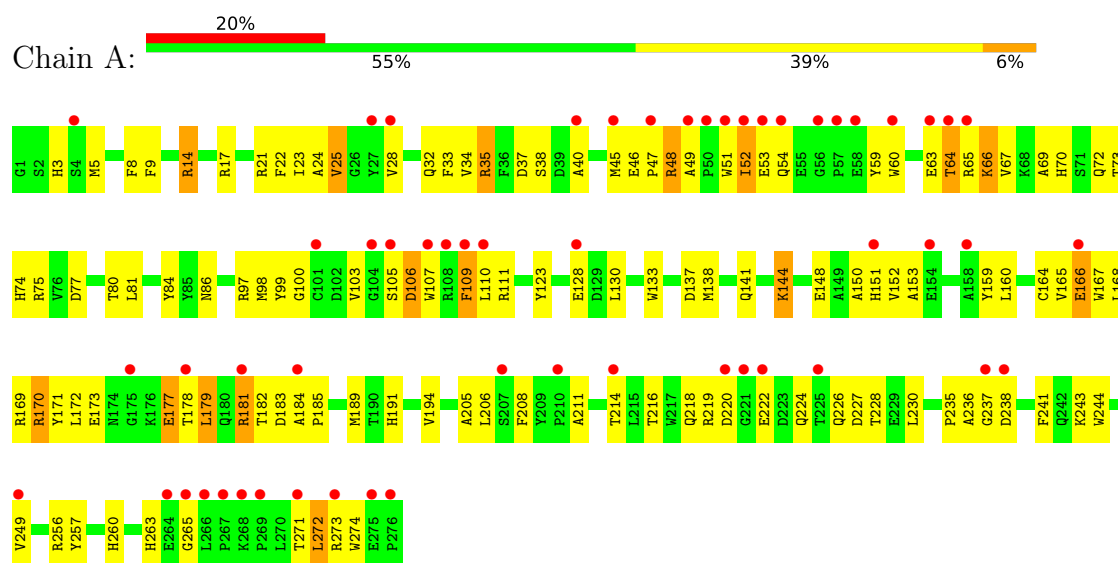
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	13	Total	O	0	0
			13	13		
6	B	14	Total	O	0	0
			14	14		
6	C	1	Total	O	0	0
			1	1		
6	D	20	Total	O	0	0
			20	20		

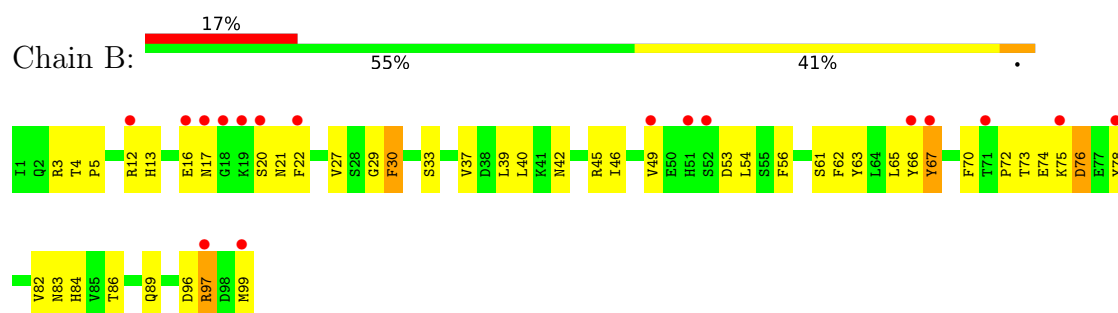
3 Residue-property plots [i](#)

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.

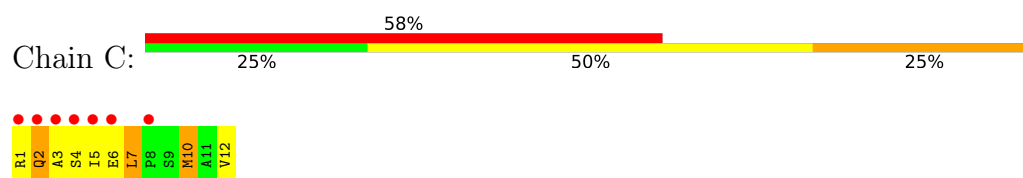
- Molecule 1: HLA class I histocompatibility antigen, A-2 alpha chain



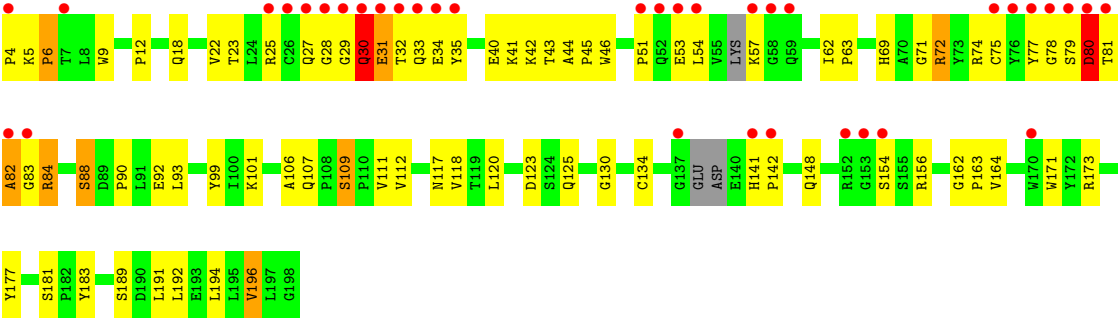
- Molecule 2: Beta-2-microglobulin



- Molecule 3: Lymphocyte-specific protein 1



- Molecule 4: Leukocyte immunoglobulin-like receptor subfamily B member 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	117.30Å 117.30Å 96.10Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.32 – 2.70 29.32 – 2.70	Depositor EDS
% Data completeness (in resolution range)	98.9 (29.32-2.70) 98.9 (29.32-2.70)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.73 (at 2.68Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.269 , 0.309 0.279 , 0.318	Depositor DCC
R_{free} test set	1080 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	48.9	Xtriage
Anisotropy	0.083	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 57.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.026 for -h,-k,l	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	4732	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.19% 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: EDO

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	0.94	2/2320 (0.1%)	1.10	16/3149 (0.5%)
2	B	1.02	1/852 (0.1%)	0.97	2/1152 (0.2%)
3	C	1.07	0/90	1.07	0/119
4	D	1.04	3/1551 (0.2%)	1.08	3/2113 (0.1%)
All	All	0.99	6/4813 (0.1%)	1.07	21/6533 (0.3%)

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
4	D	0	1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	141	HIS	CE1-NE2	6.64	1.39	1.32
1	A	46	GLU	C-N	6.04	1.41	1.33
4	D	6	PRO	N-CD	5.89	1.55	1.47
4	D	141	HIS	CG-ND1	5.88	1.44	1.38
2	B	30	PHE	CA-C	5.46	1.59	1.52
1	A	205	ALA	CA-CB	-5.20	1.45	1.53

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	194	VAL	N-CA-C	-9.59	104.14	111.90
1	A	128	GLU	N-CA-C	8.51	125.33	111.37
1	A	208	PHE	N-CA-C	8.10	122.40	110.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	109	SER	N-CA-C	8.06	115.39	108.13
1	A	48	ARG	CB-CA-C	7.97	121.57	109.13
1	A	144	LYS	N-CA-C	-7.36	103.19	111.14
1	A	181	ARG	CB-CA-C	-6.24	99.16	112.63
1	A	177	GLU	CB-CA-C	5.80	121.95	110.42
1	A	206	LEU	N-CA-C	5.77	117.38	109.18
1	A	123	TYR	CB-CA-C	-5.46	101.50	110.08
1	A	178	THR	N-CA-C	5.33	119.12	111.02
1	A	226	GLN	N-CA-C	5.30	117.14	111.36
4	D	125	GLN	N-CA-C	-5.19	106.73	113.16
1	A	14	ARG	CA-C-N	5.17	125.97	119.98
1	A	14	ARG	C-N-CA	5.17	125.97	119.98
1	A	110	LEU	N-CA-CB	5.16	119.29	110.51
1	A	66	LYS	N-CA-C	5.09	116.83	111.28
2	B	76	ASP	N-CA-C	5.09	117.41	110.24
1	A	128	GLU	CB-CA-C	-5.07	102.42	110.84
4	D	101	LYS	N-CA-C	5.06	116.26	109.83
2	B	56	PHE	N-CA-C	5.00	116.68	109.07

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	D	30	GLN	Peptide

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	2254	0	2103	116	7
2	B	829	0	794	46	0
3	C	90	0	96	24	0
4	D	1507	0	1449	56	7
5	B	4	0	6	0	0
6	A	13	0	0	1	0
6	B	14	0	0	0	0
6	C	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	D	20	0	0	0	0
All	All	4732	0	4448	219	7

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 (219) 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:97:ARG:HG2	2:B:97:ARG:HH11	1.12	1.08
3:C:6:GLU:O	3:C:7:LEU:HB2	1.57	1.01
4:D:79:SER:O	4:D:80:ASP:HB2	1.60	0.98
1:A:177:GLU:O	1:A:181:ARG:HG3	1.61	0.97
2:B:97:ARG:HH11	2:B:97:ARG:CG	1.77	0.97
2:B:97:ARG:HG2	2:B:97:ARG:NH1	1.73	0.95
1:A:182:THR:O	1:A:183:ASP:OD2	1.88	0.91
4:D:75:CYS:H	4:D:88:SER:HB3	1.38	0.86
1:A:37:ASP:HB3	1:A:40:ALA:HB2	1.57	0.85
4:D:79:SER:HB2	4:D:82:ALA:HB3	1.59	0.85
1:A:236:ALA:O	2:B:12:ARG:HG3	1.74	0.85
4:D:30:GLN:O	4:D:32:THR:HG23	1.77	0.85
2:B:70:PHE:HD2	2:B:78:TYR:CE2	1.96	0.83
1:A:109:PHE:HB2	1:A:165:VAL:HG21	1.57	0.83
1:A:28:VAL:HG23	1:A:33:PHE:CE1	2.15	0.81
3:C:10:MET:HA	3:C:10:MET:CE	2.13	0.79
1:A:52:ILE:C	1:A:54:GLN:H	1.90	0.79
2:B:33:SER:HB3	2:B:62:PHE:CE2	2.19	0.77
1:A:103:VAL:HG22	1:A:168:LEU:HD21	1.66	0.77
3:C:10:MET:HA	3:C:10:MET:HE2	1.68	0.74
1:A:109:PHE:C	1:A:109:PHE:CD2	2.66	0.74
1:A:74:HIS:HE1	1:A:97:ARG:NH1	1.86	0.73
1:A:159:TYR:CE1	3:C:2:GLN:O	2.41	0.73
3:C:6:GLU:O	3:C:7:LEU:CB	2.35	0.70
4:D:74:ARG:NH1	4:D:90:PRO:HD3	2.08	0.69
4:D:112:VAL:O	4:D:196:VAL:HA	1.93	0.69
1:A:5:MET:HB2	1:A:168:LEU:HD13	1.75	0.68
1:A:177:GLU:O	1:A:181:ARG:CG	2.42	0.66
1:A:70:HIS:ND1	3:C:5:ILE:HG21	2.11	0.66
2:B:84:HIS:CE1	2:B:86:THR:HG23	2.30	0.66
2:B:33:SER:HB3	2:B:62:PHE:CD2	2.32	0.65
1:A:159:TYR:CZ	3:C:2:GLN:O	2.49	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:79:SER:CB	4:D:82:ALA:HB3	2.25	0.65
1:A:52:ILE:C	1:A:54:GLN:N	2.56	0.64
1:A:74:HIS:CE1	1:A:97:ARG:NH1	2.65	0.64
1:A:52:ILE:O	1:A:54:GLN:N	2.30	0.64
1:A:70:HIS:HA	3:C:5:ILE:HG22	1.79	0.64
1:A:106:ASP:N	1:A:106:ASP:OD2	2.31	0.63
2:B:46:ILE:O	2:B:49:VAL:HG23	1.99	0.63
1:A:81:LEU:HD21	3:C:12:VAL:HG21	1.81	0.62
4:D:51:PRO:HG2	4:D:54:LEU:HD12	1.81	0.62
1:A:103:VAL:CG2	1:A:168:LEU:HD21	2.29	0.61
2:B:70:PHE:CD2	2:B:78:TYR:CE2	2.85	0.61
1:A:271:THR:C	1:A:272:LEU:HD23	2.25	0.61
1:A:51:TRP:H	1:A:51:TRP:CD1	2.19	0.61
1:A:74:HIS:HE1	1:A:97:ARG:HH12	1.48	0.60
2:B:73:THR:HG22	2:B:75:LYS:H	1.66	0.60
1:A:244:TRP:HE1	2:B:99:MET:HG3	1.66	0.60
1:A:219:ARG:O	1:A:220:ASP:HB2	2.03	0.59
1:A:249:VAL:HG13	1:A:257:TYR:CE1	2.38	0.59
1:A:22:PHE:HB3	1:A:38:SER:HB3	1.83	0.59
4:D:32:THR:O	4:D:35:TYR:CE1	2.57	0.58
4:D:112:VAL:HG11	4:D:118:VAL:HB	1.85	0.58
4:D:32:THR:O	4:D:35:TYR:CZ	2.57	0.58
2:B:67:TYR:N	2:B:67:TYR:CD1	2.72	0.58
2:B:16:GLU:O	2:B:72:PRO:HG2	2.04	0.57
2:B:67:TYR:H	2:B:67:TYR:HD1	1.50	0.57
2:B:29:GLY:HA2	2:B:61:SER:HB2	1.87	0.57
2:B:39:LEU:C	2:B:40:LEU:HD23	2.30	0.57
1:A:166:GLU:HG3	1:A:169:ARG:HH21	1.70	0.57
4:D:79:SER:O	4:D:80:ASP:CB	2.42	0.57
1:A:133:TRP:NE1	1:A:153:ALA:HB2	2.20	0.56
4:D:111:VAL:O	4:D:111:VAL:HG23	2.05	0.56
1:A:74:HIS:CE1	1:A:97:ARG:HH12	2.21	0.56
2:B:27:VAL:HG23	2:B:27:VAL:O	2.06	0.56
1:A:22:PHE:HE2	1:A:67:VAL:HG22	1.70	0.56
4:D:83:GLY:O	4:D:84:ARG:HB2	2.06	0.56
1:A:130:LEU:HD13	1:A:160:LEU:HD12	1.87	0.56
1:A:81:LEU:CD2	3:C:12:VAL:HG21	2.35	0.56
1:A:159:TYR:HD2	1:A:160:LEU:HD23	1.71	0.55
3:C:10:MET:CE	3:C:10:MET:CA	2.84	0.55
1:A:189:MET:HE1	1:A:274:TRP:HB2	1.89	0.55
2:B:96:ASP:O	2:B:97:ARG:C	2.48	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:9:PHE:CE2	1:A:99:TYR:CE2	2.95	0.55
2:B:12:ARG:HB2	2:B:22:PHE:HB2	1.88	0.55
1:A:45:MET:H	1:A:64:THR:HG1	1.54	0.55
1:A:170:ARG:HG3	1:A:170:ARG:HH11	1.72	0.55
1:A:103:VAL:HG13	1:A:168:LEU:HD23	1.88	0.54
4:D:28:GLY:O	4:D:30:GLN:N	2.39	0.54
1:A:21:ARG:NH2	1:A:37:ASP:OD1	2.37	0.54
1:A:35:ARG:O	1:A:35:ARG:HG3	2.06	0.54
4:D:28:GLY:C	4:D:30:GLN:N	2.66	0.54
4:D:72:ARG:HG2	4:D:92:GLU:HG2	1.89	0.54
1:A:9:PHE:HE2	1:A:99:TYR:CE2	2.26	0.54
1:A:159:TYR:CD2	1:A:160:LEU:HD23	2.43	0.54
2:B:12:ARG:NH1	2:B:22:PHE:CE2	2.76	0.54
4:D:78:GLY:CA	4:D:83:GLY:HA3	2.38	0.54
1:A:107:TRP:O	1:A:169:ARG:HD3	2.09	0.53
4:D:53:GLU:O	4:D:57:LYS:HG3	2.08	0.53
1:A:211:ALA:HB2	1:A:241:PHE:CE2	2.44	0.53
1:A:59:TYR:HE2	1:A:167:TRP:CZ3	2.26	0.53
1:A:77:ASP:OD1	3:C:12:VAL:HG22	2.08	0.53
4:D:43:THR:O	4:D:45:PRO:HD3	2.09	0.53
1:A:103:VAL:CG1	1:A:168:LEU:HD23	2.39	0.53
2:B:40:LEU:HD22	2:B:45:ARG:HA	1.90	0.53
1:A:159:TYR:OH	3:C:1:ARG:O	2.26	0.53
2:B:73:THR:HG22	2:B:74:GLU:N	2.23	0.53
4:D:171:TRP:HB3	4:D:191:LEU:HD11	1.91	0.52
1:A:184:ALA:HB2	1:A:265:GLY:O	2.09	0.52
1:A:103:VAL:CG1	1:A:165:VAL:HG13	2.38	0.52
1:A:191:HIS:HB2	1:A:274:TRP:CH2	2.44	0.52
4:D:112:VAL:CG2	4:D:164:VAL:HG21	2.39	0.52
2:B:37:VAL:HB	2:B:66:TYR:CE2	2.44	0.52
4:D:112:VAL:HG21	4:D:164:VAL:HG21	1.92	0.52
1:A:59:TYR:CE2	1:A:167:TRP:CZ3	2.98	0.52
1:A:271:THR:O	1:A:272:LEU:HD23	2.10	0.52
1:A:33:PHE:CD2	1:A:34:VAL:HG13	2.45	0.51
1:A:107:TRP:CZ2	1:A:172:LEU:HD13	2.46	0.51
1:A:224:GLN:O	1:A:228:THR:OG1	2.27	0.51
4:D:71:GLY:HA2	4:D:183:TYR:CD1	2.46	0.51
4:D:4:PRO:O	4:D:5:LYS:HB2	2.09	0.51
1:A:45:MET:HE2	3:C:2:GLN:NE2	2.26	0.50
1:A:25:VAL:HG23	1:A:32:GLN:HG3	1.94	0.50
4:D:117:ASN:ND2	4:D:163:PRO:HA	2.27	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:230:LEU:HD22	1:A:243:LYS:HE3	1.93	0.50
4:D:106:ALA:HA	4:D:120:LEU:HD23	1.93	0.50
2:B:29:GLY:HA2	2:B:61:SER:CB	2.40	0.50
1:A:23:ILE:HG12	1:A:37:ASP:OD1	2.12	0.50
1:A:137:ASP:OD1	1:A:137:ASP:C	2.54	0.50
2:B:17:ASN:ND2	2:B:97:ARG:HH21	2.10	0.50
4:D:81:THR:O	4:D:82:ALA:HB2	2.12	0.50
1:A:224:GLN:NE2	6:A:312:HOH:O	2.45	0.49
1:A:63:GLU:OE2	3:C:1:ARG:HB2	2.12	0.49
1:A:103:VAL:HG12	1:A:165:VAL:HG13	1.94	0.49
4:D:78:GLY:HA2	4:D:83:GLY:HA3	1.94	0.49
4:D:22:VAL:HG13	4:D:62:ILE:HD12	1.94	0.49
4:D:72:ARG:HG3	4:D:183:TYR:OH	2.13	0.49
2:B:21:ASN:HB3	2:B:70:PHE:CE1	2.47	0.49
1:A:80:THR:HG22	1:A:84:TYR:CE1	2.48	0.49
1:A:33:PHE:O	1:A:48:ARG:N	2.46	0.49
1:A:49:ALA:HB1	1:A:51:TRP:NE1	2.28	0.49
2:B:12:ARG:CB	2:B:22:PHE:HB2	2.43	0.48
1:A:59:TYR:CE2	1:A:167:TRP:HZ3	2.32	0.48
1:A:218:GLN:CD	1:A:260:HIS:NE2	2.72	0.48
1:A:152:VAL:HG13	3:C:10:MET:HE1	1.95	0.48
3:C:10:MET:CA	3:C:10:MET:HE3	2.44	0.48
2:B:17:ASN:HD21	2:B:97:ARG:HH21	1.61	0.48
2:B:67:TYR:N	2:B:67:TYR:HD1	2.11	0.47
4:D:173:ARG:HD3	4:D:189:SER:O	2.14	0.47
1:A:144:LYS:O	1:A:148:GLU:HG2	2.13	0.47
1:A:224:GLN:OE1	1:A:224:GLN:HA	2.15	0.47
1:A:133:TRP:HE1	1:A:153:ALA:HB2	1.78	0.47
2:B:13:HIS:C	2:B:21:ASN:HD21	2.23	0.47
4:D:9:TRP:CE2	4:D:25:ARG:HB2	2.49	0.47
1:A:184:ALA:HB1	1:A:185:PRO:HD2	1.97	0.47
4:D:9:TRP:CZ2	4:D:25:ARG:HB3	2.51	0.46
4:D:123:ASP:OD2	4:D:156:ARG:HB2	2.16	0.46
1:A:3:HIS:HB2	1:A:103:VAL:HG23	1.96	0.46
2:B:42:ASN:HD21	2:B:76:ASP:HA	1.81	0.46
2:B:53:ASP:O	2:B:54:LEU:C	2.58	0.46
4:D:34:GLU:O	4:D:77:TYR:HA	2.16	0.46
2:B:89:GLN:NE2	4:D:18:GLN:OE1	2.49	0.46
1:A:150:ALA:O	1:A:151:HIS:HB2	2.15	0.45
1:A:28:VAL:HG23	1:A:33:PHE:HE1	1.76	0.45
1:A:28:VAL:CG2	1:A:33:PHE:CE1	2.94	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:47:PRO:HB3	1:A:60:TRP:CZ2	2.51	0.45
1:A:235:PRO:HG2	2:B:65:LEU:HD22	1.99	0.45
1:A:263:HIS:CE1	1:A:265:GLY:H	2.34	0.45
1:A:5:MET:HE2	1:A:164:CYS:SG	2.57	0.45
1:A:72:GLN:O	1:A:75:ARG:HB3	2.16	0.45
1:A:168:LEU:O	1:A:171:TYR:N	2.50	0.45
2:B:29:GLY:C	2:B:61:SER:HB2	2.42	0.45
1:A:237:GLY:O	2:B:12:ARG:NH2	2.49	0.45
1:A:3:HIS:HB2	1:A:103:VAL:CG2	2.47	0.45
1:A:47:PRO:HB3	1:A:60:TRP:CH2	2.52	0.45
4:D:28:GLY:C	4:D:30:GLN:H	2.23	0.45
1:A:37:ASP:HB3	1:A:40:ALA:CB	2.37	0.44
1:A:23:ILE:HG22	1:A:24:ALA:N	2.33	0.44
2:B:13:HIS:HB2	2:B:21:ASN:OD1	2.17	0.44
4:D:117:ASN:ND2	4:D:162:GLY:HA3	2.33	0.44
4:D:75:CYS:O	4:D:88:SER:N	2.39	0.44
1:A:165:VAL:HG12	1:A:169:ARG:CZ	2.47	0.44
1:A:70:HIS:CE1	3:C:5:ILE:HG21	2.53	0.44
1:A:220:ASP:OD2	1:A:256:ARG:NH2	2.48	0.44
1:A:5:MET:O	1:A:100:GLY:HA3	2.17	0.44
4:D:62:ILE:HA	4:D:63:PRO:HD2	1.87	0.43
1:A:28:VAL:HG23	1:A:33:PHE:CD1	2.52	0.43
2:B:29:GLY:HA2	2:B:61:SER:OG	2.19	0.43
2:B:63:TYR:CD1	2:B:63:TYR:C	2.96	0.43
4:D:42:LYS:HB2	4:D:42:LYS:HE3	1.85	0.43
4:D:44:ALA:HB1	4:D:46:TRP:CD1	2.53	0.43
4:D:62:ILE:O	4:D:63:PRO:C	2.61	0.43
4:D:134:CYS:HB3	4:D:142:PRO:HB3	2.01	0.43
1:A:77:ASP:OD1	3:C:12:VAL:HG13	2.19	0.43
4:D:69:HIS:O	4:D:93:LEU:HD23	2.19	0.42
4:D:118:VAL:HG11	4:D:194:LEU:HD11	2.01	0.42
1:A:70:HIS:CG	3:C:5:ILE:HG21	2.54	0.42
4:D:117:ASN:HD22	4:D:163:PRO:HA	1.83	0.42
1:A:66:LYS:O	1:A:69:ALA:HB3	2.19	0.42
1:A:97:ARG:HG2	1:A:98:MET:N	2.34	0.42
1:A:45:MET:N	1:A:64:THR:OG1	2.39	0.42
1:A:138:MET:SD	1:A:141:GLN:NE2	2.92	0.42
4:D:111:VAL:O	4:D:111:VAL:CG2	2.66	0.42
4:D:51:PRO:CG	4:D:54:LEU:HD12	2.48	0.42
1:A:37:ASP:O	1:A:40:ALA:HB3	2.19	0.42
1:A:179:LEU:H	1:A:179:LEU:HG	1.66	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:2:GLN:HB3	3:C:3:ALA:H	1.64	0.42
4:D:30:GLN:O	4:D:32:THR:N	2.51	0.42
1:A:69:ALA:HB1	3:C:6:GLU:HA	2.02	0.42
1:A:81:LEU:HA	1:A:84:TYR:HB2	2.02	0.42
1:A:8:PHE:CE2	1:A:98:MET:HG3	2.55	0.41
2:B:5:PRO:HB3	2:B:30:PHE:HB3	2.02	0.41
2:B:84:HIS:ND1	2:B:86:THR:HG23	2.34	0.41
2:B:82:VAL:HG12	2:B:83:ASN:N	2.36	0.41
1:A:73:THR:HA	3:C:7:LEU:HD13	2.03	0.41
2:B:29:GLY:CA	2:B:61:SER:HB2	2.51	0.41
1:A:52:ILE:HD12	1:A:52:ILE:HA	1.76	0.41
1:A:14:ARG:HB3	1:A:17:ARG:HB2	2.01	0.41
1:A:165:VAL:O	1:A:168:LEU:HB3	2.20	0.41
4:D:40:GLU:O	4:D:41:LYS:HB2	2.20	0.41
4:D:51:PRO:HB2	4:D:53:GLU:CG	2.50	0.41
1:A:33:PHE:HD2	1:A:34:VAL:HG13	1.85	0.41
4:D:22:VAL:HG22	4:D:23:THR:N	2.35	0.41
4:D:31:GLU:H	4:D:31:GLU:HG3	1.40	0.41
4:D:130:GLY:HA3	4:D:177:TYR:CZ	2.56	0.41
1:A:159:TYR:OH	3:C:2:GLN:O	2.37	0.40
1:A:236:ALA:C	2:B:12:ARG:HG3	2.44	0.40
1:A:5:MET:CE	1:A:164:CYS:SG	3.09	0.40
2:B:73:THR:CG2	2:B:74:GLU:N	2.85	0.40

All (7) 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:A:65:ARG:NH2	4:D:80:ASP:O[4_655]	1.20	1.00
1:A:65:ARG:NH2	4:D:80:ASP:C[4_655]	1.30	0.90
1:A:65:ARG:CZ	4:D:80:ASP:O[4_655]	1.63	0.57
1:A:65:ARG:NE	4:D:80:ASP:O[4_655]	1.95	0.25
1:A:65:ARG:NE	4:D:81:THR:CA[4_655]	1.97	0.23
1:A:65:ARG:NH2	4:D:81:THR:N[4_655]	2.02	0.18
1:A:65:ARG:CZ	4:D:81:THR:CA[4_655]	2.17	0.03

5.3 Torsion angles

5.3.1 Protein backbone

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	274/276 (99%)	242 (88%)	31 (11%)	1 (0%)	30	54
2	B	97/99 (98%)	90 (93%)	7 (7%)	0	100	100
3	C	10/12 (83%)	5 (50%)	2 (20%)	3 (30%)	0	0
4	D	186/195 (95%)	167 (90%)	13 (7%)	6 (3%)	3	7
All	All	567/582 (97%)	504 (89%)	53 (9%)	10 (2%)	6	18

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	53	GLU
3	C	2	GLN
3	C	4	SER
4	D	6	PRO
4	D	80	ASP
4	D	82	ALA
4	D	84	ARG
4	D	29	GLY
3	C	7	LEU
4	D	12	PRO

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	232/232 (100%)	212 (91%)	20 (9%)	10	25

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	94/94 (100%)	89 (95%)	5 (5%)	20	46
3	C	10/10 (100%)	9 (90%)	1 (10%)	7	19
4	D	166/169 (98%)	151 (91%)	15 (9%)	9	23
All	All	502/505 (99%)	461 (92%)	41 (8%)	10	27

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	VAL
1	A	35	ARG
1	A	52	ILE
1	A	64	THR
1	A	86	ASN
1	A	105	SER
1	A	106	ASP
1	A	109	PHE
1	A	111	ARG
1	A	166	GLU
1	A	170	ARG
1	A	173	GLU
1	A	179	LEU
1	A	214	THR
1	A	216	THR
1	A	222	GLU
1	A	227	ASP
1	A	238	ASP
1	A	272	LEU
1	A	273	ARG
2	B	3	ARG
2	B	4	THR
2	B	20	SER
2	B	67	TYR
2	B	97	ARG
3	C	10	MET
4	D	27	GLN
4	D	30	GLN
4	D	31	GLU
4	D	33	GLN
4	D	72	ARG
4	D	80	ASP
4	D	88	SER

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Mol	Chain	Res	Type
4	D	99	TYR
4	D	107	GLN
4	D	109	SER
4	D	148	GLN
4	D	154	SER
4	D	181	SER
4	D	192	LEU
4	D	196	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	72	GLN
1	A	74	HIS
1	A	86	ASN
1	A	87	GLN
1	A	174	ASN
1	A	218	GLN
1	A	226	GLN
2	B	2	GLN
2	B	17	ASN
2	B	42	ASN
2	B	89	GLN
4	D	113	ASN
4	D	117	ASN
4	D	125	GLN
4	D	148	GLN
4	D	180	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

1 ligand is 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	$\# Z > 2$
5	EDO	B	101	-	3,3,3	1.11	0	2,2,2	0.24	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
5	EDO	B	101	-	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	101	EDO	O1-C1-C2-O2

There are no ring outliers.

No monomer is involved in short contacts.

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(Å²)	Q<0.9
1	A	276/276 (100%)	1.13	55 (19%)	3	2	12, 54, 96, 112	13 (4%)
2	B	99/99 (100%)	0.78	17 (17%)	4	3	17, 41, 75, 96	6 (6%)
3	C	12/12 (100%)	2.30	7 (58%)	0	0	58, 73, 109, 114	0
4	D	192/195 (98%)	0.78	36 (18%)	3	3	16, 49, 107, 130	7 (3%)
All	All	579/582 (99%)	0.98	115 (19%)	3	2	12, 50, 98, 130	26 (4%)

All (115) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	D	32	THR	5.5
1	A	56	GLY	5.0
1	A	63	GLU	4.9
4	D	7	THR	4.9
2	B	99	MET	4.9
1	A	151	HIS	4.9
1	A	268	LYS	4.8
1	A	184	ALA	4.7
3	C	3	ALA	4.7
2	B	51	HIS	4.6
1	A	225	THR	4.3
1	A	64	THR	4.2
1	A	158	ALA	4.2
1	A	265	GLY	4.2
4	D	79	SER	4.2
1	A	108	ARG	4.1
2	B	12	ARG	4.1
4	D	33	GLN	4.1
1	A	105	SER	4.1
3	C	1	ARG	4.0
3	C	6	GLU	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	28	VAL	3.8
4	D	78	GLY	3.7
1	A	109	PHE	3.7
4	D	31	GLU	3.7
1	A	104	GLY	3.6
1	A	53	GLU	3.5
2	B	18	GLY	3.4
1	A	207	SER	3.3
4	D	35	TYR	3.3
1	A	210	PRO	3.3
4	D	4	PRO	3.3
4	D	142	PRO	3.3
1	A	52	ILE	3.3
1	A	110	LEU	3.2
1	A	154	GLU	3.2
4	D	51	PRO	3.2
4	D	54	LEU	3.2
4	D	30	GLN	3.2
2	B	19	LYS	3.1
4	D	152	ARG	3.1
1	A	178	THR	3.1
1	A	275	GLU	3.1
1	A	54	GLN	3.1
4	D	137	GLY	3.0
2	B	52	SER	3.0
1	A	276	PRO	3.0
4	D	83	GLY	3.0
4	D	77	TYR	3.0
4	D	34	GLU	2.9
2	B	78	TYR	2.9
1	A	65	ARG	2.8
2	B	67	TYR	2.8
1	A	181	ARG	2.8
2	B	97	ARG	2.8
4	D	59	GLN	2.8
1	A	47	PRO	2.8
4	D	52	GLN	2.8
1	A	221	GLY	2.7
4	D	28	GLY	2.7
1	A	166	GLU	2.7
1	A	267	PRO	2.7
1	A	107	TRP	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	60	TRP	2.7
1	A	214	THR	2.7
1	A	269	PRO	2.6
1	A	40	ALA	2.6
1	A	50	PRO	2.6
4	D	81	THR	2.5
1	A	45	MET	2.5
1	A	264	GLU	2.5
4	D	29	GLY	2.5
4	D	26	CYS	2.5
1	A	238	ASP	2.5
1	A	273	ARG	2.5
2	B	20	SER	2.5
1	A	51	TRP	2.5
1	A	58	GLU	2.4
1	A	266	LEU	2.4
2	B	16	GLU	2.4
1	A	271	THR	2.3
4	D	76	TYR	2.3
4	D	154	SER	2.3
1	A	237	GLY	2.3
4	D	27	GLN	2.3
1	A	128	GLU	2.3
3	C	4	SER	2.3
4	D	58	GLY	2.3
4	D	75	CYS	2.2
1	A	27	TYR	2.2
1	A	4	SER	2.2
2	B	17	ASN	2.2
4	D	170	TRP	2.2
1	A	101	CYS	2.2
1	A	222	GLU	2.2
4	D	57	LYS	2.2
4	D	53	GLU	2.1
2	B	71	THR	2.1
3	C	8	PRO	2.1
4	D	153	GLY	2.1
4	D	80	ASP	2.1
2	B	22	PHE	2.1
1	A	49	ALA	2.1
2	B	66	TYR	2.1
4	D	25	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
3	C	2	GLN	2.1
1	A	220	ASP	2.1
4	D	141	HIS	2.1
3	C	5	ILE	2.1
2	B	49	VAL	2.1
2	B	75	LYS	2.0
4	D	82	ALA	2.0
1	A	57	PRO	2.0
1	A	175	GLY	2.0
1	A	249	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
5	EDO	B	101	4/4	0.89	0.15	56,56,56,56	0

6.5 Other polymers [i](#)

There are no such residues in this entry.