



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 01:30 AM UTC

PDB ID : 2PCP / pdb_00002pcp
Title : ANTIBODY FAB COMPLEXED WITH PHENCYCLIDINE
Authors : Lim, K.; Owens, S.M.; Arnold, L.; Sacchettini, J.C.; Linthicum, D.S.
Deposited on : 1998-06-02
Resolution : 2.20 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

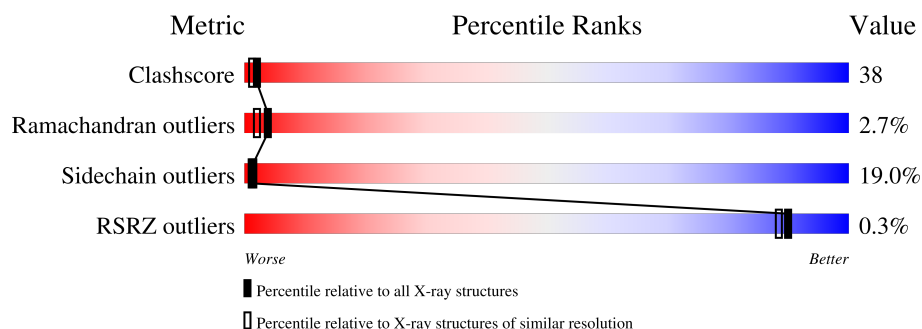
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	216	32% 59% 8% .
1	C	216	31% 53% 15%
2	B	215	27% 53% 17% .
2	D	215	% 36% 51% 13%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 7342 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 IMMUNOGLOBULIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	216	Total	C	N	O	S	0	0	0
			1678	1051	283	338	6			
1	C	216	Total	C	N	O	S	0	0	0
			1678	1051	283	338	6			

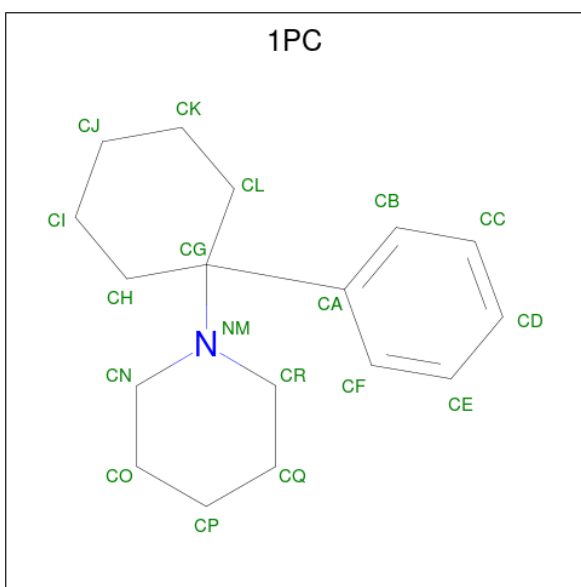
There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	27A	THR	SER	conflict	PIR PC4203
A	27E	SER	THR	conflict	PIR PC4203
A	52	THR	SER	conflict	PIR PC4203
A	92	THR	SER	conflict	PIR PC4203
A	94	ALA	VAL	conflict	PIR PC4203
A	96	TYR	ARG	conflict	PIR PC4203
C	27A	THR	SER	conflict	PIR PC4203
C	27E	SER	THR	conflict	PIR PC4203
C	52	THR	SER	conflict	PIR PC4203
C	92	THR	SER	conflict	PIR PC4203
C	94	ALA	VAL	conflict	PIR PC4203
C	96	TYR	ARG	conflict	PIR PC4203

- Molecule 2 is a protein called IMMUNOGLOBULIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	215	Total	C	N	O	S	0	0	0
			1636	1033	268	328	7			
2	D	215	Total	C	N	O	S	0	0	0
			1636	1033	268	328	7			

- Molecule 3 is 1-(PHENYL-1-CYCLOHEXYL)PIPERIDINE (CCD ID: 1PC) (formula: C₁₇H₂₅N).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	N	0	0
			18	17	1		
3	C	1	Total	C	N	0	0
			18	17	1		

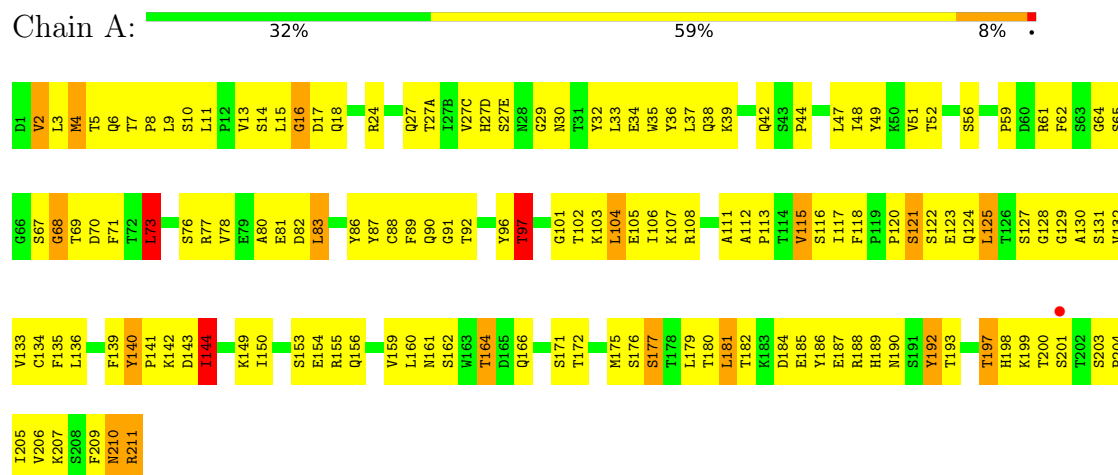
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	173	Total	O	0	0
			173	173		
4	B	163	Total	O	0	0
			163	163		
4	C	150	Total	O	0	0
			150	150		
4	D	192	Total	O	0	0
			192	192		

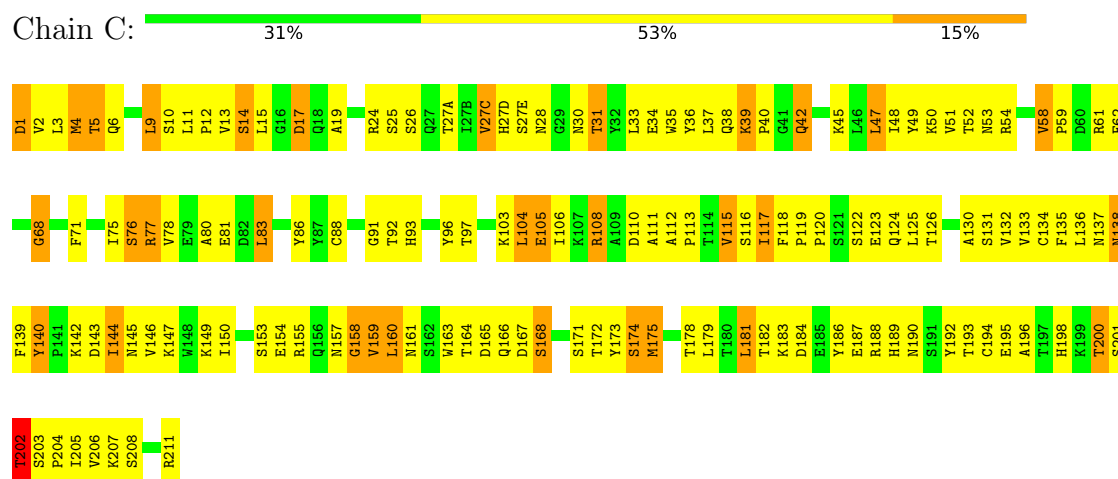
3 Residue-property plots

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.

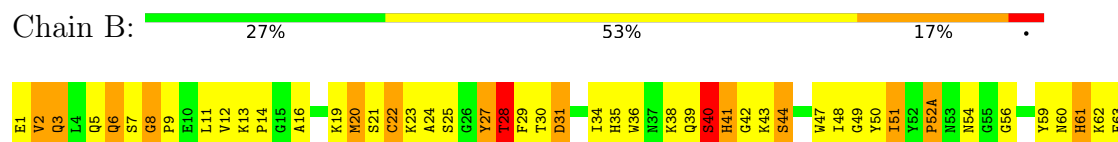
• Molecule 1: IMMUNOGLOBULIN

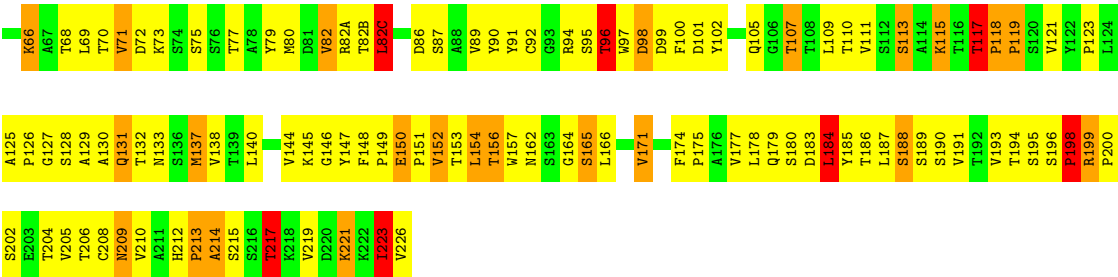


• Molecule 1: IMMUNOGLOBULIN

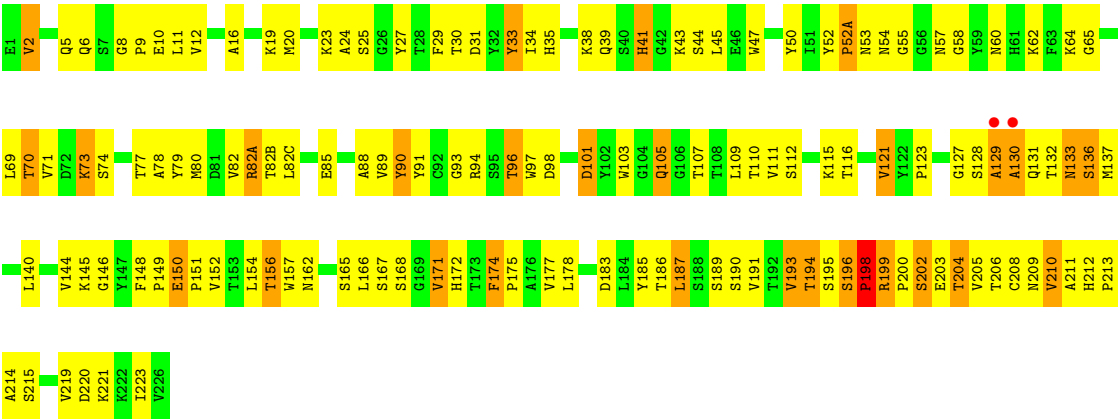


• Molecule 2: IMMUNOGLOBULIN





● Molecule 2: IMMUNOGLOBULIN



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	53.46Å 67.72Å 68.04Å 62.11° 84.66° 83.17°	Depositor
Resolution (Å)	6.00 – 2.20 6.00 – 2.20	Depositor EDS
% Data completeness (in resolution range)	78.7 (6.00-2.20) 74.9 (6.00-2.20)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.51 (at 2.08Å)	Xtriage
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.196 , 0.290 0.208 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	20.8	Xtriage
Anisotropy	0.418	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 142.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.109 for -h,-l,-k	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	7342	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.25% 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: 1PC

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	0.88	1/1717 (0.1%)	1.30	18/2330 (0.8%)
1	C	0.95	2/1717 (0.1%)	1.37	26/2330 (1.1%)
2	B	0.97	2/1681 (0.1%)	1.38	25/2295 (1.1%)
2	D	0.92	1/1681 (0.1%)	1.50	30/2295 (1.3%)
All	All	0.93	6/6796 (0.1%)	1.39	99/9250 (1.1%)

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	A	0	2
1	C	0	1
2	B	0	1
2	D	0	2
All	All	0	6

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	196	ALA	CA-CB	-7.26	1.43	1.53
2	B	51	ILE	CA-CB	6.90	1.63	1.55
1	C	204	PRO	CA-C	-5.90	1.46	1.52
1	A	4	MET	SD-CE	-5.53	1.65	1.79
2	B	28	THR	CA-CB	5.31	1.59	1.52
2	D	2	VAL	CA-CB	5.02	1.61	1.54

All (99) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	129	ALA	N-CA-C	-14.21	85.02	108.32
2	D	128	SER	N-CA-C	11.08	126.20	109.25
2	D	150	GLU	CA-C-N	-9.77	107.63	119.84
2	D	150	GLU	C-N-CA	-9.77	107.63	119.84
1	A	201	SER	N-CA-C	-9.35	93.66	108.90
1	C	124	GLN	N-CA-C	9.13	122.21	111.71
1	A	205	ILE	N-CA-C	-8.86	94.58	107.78
2	D	55	GLY	N-CA-C	-8.86	102.44	115.63
2	D	10	GLU	N-CA-C	8.66	122.16	109.69
2	D	145	LYS	N-CA-C	8.65	123.33	109.24
2	D	130	ALA	N-CA-C	8.57	129.06	110.80
2	B	133	ASN	N-CA-C	8.54	123.51	113.18
1	C	39	LYS	N-CA-C	-8.16	99.78	110.07
2	B	117	THR	CA-C-N	7.97	128.59	120.38
2	B	117	THR	C-N-CA	7.97	128.59	120.38
2	D	204	THR	N-CA-C	7.92	122.71	110.20
1	C	58	VAL	CA-C-N	7.88	127.83	120.03
1	C	58	VAL	C-N-CA	7.88	127.83	120.03
2	B	150	GLU	CA-C-N	-7.64	110.29	119.84
2	B	150	GLU	C-N-CA	-7.64	110.29	119.84
2	B	96	THR	N-CA-C	-7.57	100.77	110.53
1	C	42	GLN	N-CA-C	7.50	120.47	109.07
1	A	105	GLU	N-CA-C	-7.44	99.51	110.52
2	B	217	THR	N-CA-C	7.39	120.84	108.20
2	D	73	LYS	N-CA-C	7.35	120.34	111.82
1	C	174	SER	N-CA-C	-7.31	97.96	109.07
1	C	106	ILE	CB-CA-C	-7.24	102.61	111.08
2	B	6	GLN	N-CA-C	-7.20	97.86	109.96
2	D	127	GLY	N-CA-C	-7.18	101.23	112.58
2	B	7	SER	N-CA-C	7.11	118.55	108.74
2	B	60	ASN	N-CA-C	-7.06	98.54	109.76
2	D	136	SER	N-CA-C	-7.05	103.73	114.16
1	A	122	SER	N-CA-C	7.04	118.60	111.07
2	B	31	ASP	N-CA-C	6.95	121.01	112.54
2	D	121	VAL	N-CA-C	6.93	118.84	108.23
2	D	150	GLU	N-CA-C	6.89	125.05	109.81
2	D	8	GLY	N-CA-C	6.81	126.24	112.34
1	A	73	LEU	N-CA-C	-6.78	98.64	109.76
1	C	119	PRO	N-CA-C	-6.70	102.52	110.70
2	B	8	GLY	N-CA-C	6.66	125.92	112.34
2	D	165	SER	N-CA-C	-6.60	96.74	110.80
1	C	158	GLY	N-CA-C	-6.56	104.32	115.08
2	B	34	ILE	N-CA-C	-6.51	99.08	108.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	27	TYR	N-CA-C	6.44	116.56	108.45
1	A	112	ALA	CA-C-N	6.36	126.58	119.90
1	A	112	ALA	C-N-CA	6.36	126.58	119.90
2	B	40	SER	N-CA-C	6.30	119.83	108.17
2	D	44	SER	N-CA-C	6.27	119.62	109.40
1	A	164	THR	N-CA-C	-6.25	101.27	110.52
1	A	52	THR	N-CA-C	6.20	121.13	113.50
2	D	171	VAL	N-CA-C	6.16	117.00	109.30
1	C	108	ARG	N-CA-C	6.12	116.09	108.19
1	C	76	SER	N-CA-C	-6.10	99.25	108.96
1	A	128	GLY	N-CA-C	6.09	123.54	114.95
1	C	200	THR	N-CA-C	6.09	123.77	110.80
1	C	171	SER	N-CA-C	6.05	120.21	111.56
2	B	153	THR	N-CA-CB	5.96	119.94	110.57
2	D	128	SER	CA-C-N	5.96	131.78	121.64
2	D	128	SER	C-N-CA	5.96	131.78	121.64
2	B	98	ASP	N-CA-C	5.92	120.68	112.45
1	C	48	ILE	N-CA-C	5.90	116.43	108.17
2	B	164	GLY	N-CA-C	-5.88	106.98	115.27
1	C	27(C)	VAL	N-CA-C	-5.86	101.15	108.89
2	D	2	VAL	N-CA-C	-5.84	99.90	109.12
1	C	97	THR	N-CA-C	5.82	119.05	109.85
1	A	115	VAL	N-CA-C	5.80	116.94	108.58
2	D	31	ASP	N-CA-C	5.78	120.06	112.89
1	C	105	GLU	N-CA-C	5.76	117.80	108.41
1	C	30	ASN	N-CA-C	-5.73	100.45	109.50
1	C	202	THR	CA-C-N	-5.73	114.88	122.56
1	C	202	THR	C-N-CA	-5.73	114.88	122.56
1	C	159	VAL	CB-CA-C	-5.73	102.63	110.77
1	A	16	GLY	N-CA-C	-5.73	107.77	115.21
2	B	110	THR	CB-CA-C	-5.71	100.93	110.19
2	B	99	ASP	N-CA-C	5.69	117.72	109.07
1	A	177	SER	N-CA-C	-5.66	99.67	108.90
2	D	193	VAL	N-CA-C	5.64	116.30	108.23
1	A	51	VAL	N-CA-C	5.63	121.05	109.34
2	D	220	ASP	N-CA-C	-5.62	99.56	108.73
2	D	58	GLY	N-CA-C	-5.58	101.09	111.14
2	D	101	ASP	N-CA-C	-5.51	104.19	111.96
2	B	9	PRO	N-CA-C	-5.51	102.48	111.68
1	A	197	THR	N-CA-C	-5.50	102.37	110.52
2	D	41	HIS	N-CA-C	5.47	117.31	110.91
2	B	51	ILE	N-CA-C	-5.42	101.12	108.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	184	LEU	N-CA-C	-5.42	101.28	109.85
2	D	183	ASP	N-CA-C	5.39	119.14	112.24
2	B	205	VAL	N-CA-C	-5.31	100.00	107.75
1	C	201	SER	N-CA-C	5.30	122.08	110.80
1	C	138	ASN	N-CA-C	5.29	122.08	110.80
1	C	202	THR	N-CA-C	5.25	121.97	110.80
1	C	47	LEU	N-CA-C	-5.24	103.05	111.02
2	B	221	LYS	N-CA-C	5.23	117.81	109.81
1	A	106	ILE	N-CA-C	5.17	115.51	107.28
1	A	68	GLY	N-CA-C	5.13	125.35	113.18
2	D	144	VAL	CB-CA-C	-5.13	106.83	112.68
1	C	115	VAL	N-CA-C	5.08	116.12	109.21
1	A	97	THR	N-CA-C	5.03	118.27	110.17
2	D	174	PHE	N-CA-C	5.02	117.00	110.08

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	140	TYR	Sidechain
1	A	192	TYR	Sidechain
2	B	50	TYR	Sidechain
1	C	140	TYR	Sidechain
2	D	50	TYR	Sidechain
2	D	90	TYR	Sidechain

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	1678	0	1621	128	0
1	C	1678	0	1621	122	0
2	B	1636	0	1578	166	0
2	D	1636	0	1578	115	0
3	B	18	0	25	5	0
3	C	18	0	25	8	0
4	A	173	0	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	163	0	0	6	0
4	C	150	0	0	4	0
4	D	192	0	0	8	0
All	All	7342	0	6448	494	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 38.

All (494) 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:190:ASN:HB2	1:C:203:SER:HB2	1.31	1.10
1:A:8:PRO:HG3	1:A:11:LEU:HD13	1.36	1.07
2:B:199:ARG:HD2	2:B:200:PRO:HA	1.36	1.05
2:D:171:VAL:HG12	2:D:191:VAL:HG23	1.37	1.03
2:B:127:GLY:HA2	2:D:131:GLN:HB2	1.36	1.02
2:B:11:LEU:HD22	2:B:149:PRO:HG3	1.38	1.02
2:D:35:HIS:HD2	2:D:47:TRP:HE1	1.14	0.95
1:A:209:PHE:HB3	2:B:128:SER:HB3	1.51	0.92
1:C:184:ASP:HB3	1:C:188:ARG:NH2	1.86	0.90
1:A:190:ASN:CB	1:C:203:SER:HB2	2.03	0.88
2:B:194:THR:HB	2:B:198:PRO:HD2	1.58	0.85
2:D:121:VAL:HG21	2:D:210:VAL:HG21	1.57	0.85
2:D:52(A):PRO:O	2:D:73:LYS:HD3	1.76	0.84
1:A:115:VAL:HG12	1:A:207:LYS:HG3	1.60	0.83
2:B:35:HIS:HD2	2:B:47:TRP:HE1	1.20	0.83
2:B:97:TRP:O	3:B:227:1PC:HR2	1.77	0.83
1:A:140:TYR:CD1	1:A:141:PRO:HA	2.14	0.83
1:C:47:LEU:HA	1:C:58:VAL:HG21	1.61	0.82
2:B:125:ALA:HB2	2:B:223:ILE:HG21	1.62	0.82
2:B:129:ALA:O	2:D:130:ALA:HB2	1.81	0.81
2:B:154:LEU:HD12	2:B:156:THR:N	1.95	0.81
1:C:81:GLU:HB2	4:C:353:HOH:O	1.82	0.79
1:C:27(A):THR:HG23	1:C:27(C):VAL:HG23	1.63	0.79
2:B:196:SER:HB2	2:B:198:PRO:HD3	1.65	0.78
1:A:150:ILE:HD11	1:A:179:LEU:HD21	1.66	0.78
2:D:171:VAL:CG1	2:D:191:VAL:HG23	2.14	0.78
2:B:117:THR:O	2:B:147:TYR:HA	1.83	0.78
1:C:5:THR:HG22	1:C:24:ARG:HD3	1.65	0.77
1:A:108:ARG:HD2	1:A:171:SER:HB2	1.66	0.77
1:C:27(D):HIS:HD2	1:C:28:ASN:H	1.30	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:160:LEU:HD21	2:B:179:GLN:HG3	1.67	0.77
2:D:60:ASN:OD1	2:D:62:LYS:HD2	1.84	0.76
2:B:128:SER:N	2:D:130:ALA:HB3	1.99	0.76
3:C:212:1PC:HC	2:D:33:TYR:CD2	2.22	0.75
2:B:171:VAL:HG12	2:B:191:VAL:HG23	1.68	0.75
2:B:199:ARG:HH11	2:B:199:ARG:HB3	1.51	0.75
2:B:3:GLN:HG3	2:B:25:SER:HB2	1.68	0.74
1:C:186:TYR:CZ	1:C:211:ARG:HG3	2.21	0.74
1:C:4:MET:HE1	1:C:25:SER:OG	1.88	0.73
2:B:2:VAL:HG21	2:B:94:ARG:NH2	2.01	0.73
1:C:136:LEU:HD21	1:C:146:VAL:CG2	2.18	0.73
1:A:150:ILE:HG13	1:A:155:ARG:HE	1.52	0.73
1:C:118:PHE:O	1:C:132:VAL:HG13	1.89	0.73
2:B:118:PRO:HB2	4:B:311:HOH:O	1.87	0.73
2:B:127:GLY:HA2	2:D:131:GLN:CB	2.16	0.73
2:B:215:SER:HB2	2:B:217:THR:OG1	1.88	0.73
2:B:66:LYS:NZ	2:B:82:VAL:HG13	2.04	0.72
2:B:35:HIS:CD2	2:B:47:TRP:HE1	2.06	0.72
1:C:80:ALA:HB1	1:C:168:SER:O	1.90	0.71
1:A:33:LEU:HD22	1:A:71:PHE:CG	2.26	0.71
2:D:154:LEU:HD23	2:D:154:LEU:H	1.54	0.71
1:C:159:VAL:HG22	1:C:179:LEU:HD12	1.72	0.71
2:D:105:GLN:H	2:D:105:GLN:CD	1.99	0.70
2:B:199:ARG:HB3	2:B:199:ARG:NH1	2.06	0.70
1:C:27(C):VAL:HA	1:C:31:THR:HG23	1.74	0.70
1:C:96:TYR:CZ	3:C:212:1PC:HF	2.27	0.69
2:D:178:LEU:HD13	2:D:185:TYR:CE1	2.28	0.69
1:C:4:MET:HA	1:C:4:MET:CE	2.22	0.69
1:C:117:ILE:HB	1:C:207:LYS:HG2	1.73	0.69
1:C:195:GLU:HG2	1:C:206:VAL:HG22	1.75	0.69
2:D:166:LEU:H	2:D:166:LEU:HD12	1.56	0.69
1:C:142:LYS:O	1:C:144:ILE:HG22	1.93	0.69
2:B:43:LYS:HD2	2:B:44:SER:N	2.08	0.68
2:B:69:LEU:CD2	2:B:80:MET:HG3	2.24	0.68
2:B:115:LYS:H	2:B:115:LYS:HD2	1.58	0.68
1:A:144:ILE:HG13	1:A:197:THR:O	1.93	0.68
2:D:194:THR:C	2:D:198:PRO:HD2	2.19	0.68
3:C:212:1PC:HC	2:D:33:TYR:CE2	2.29	0.68
2:B:223:ILE:HG23	2:B:226:VAL:N	2.09	0.67
1:C:149:LYS:HE3	1:C:195:GLU:OE1	1.94	0.67
1:A:142:LYS:O	1:A:144:ILE:HG22	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:212:1PC:CR	2:D:97:TRP:O	2.42	0.67
2:D:199:ARG:HG2	2:D:200:PRO:HA	1.75	0.67
2:D:80:MET:HE1	2:D:90:TYR:CD2	2.29	0.67
1:A:144:ILE:HB	1:A:198:HIS:CD2	2.30	0.66
2:D:6:GLN:HB2	2:D:105:GLN:OE1	1.95	0.66
2:D:71:VAL:HG12	2:D:78:ALA:HA	1.78	0.66
2:D:20:MET:HG2	2:D:107:THR:HG21	1.76	0.66
2:B:43:LYS:HD2	2:B:44:SER:H	1.60	0.66
2:B:115:LYS:NZ	2:B:115:LYS:HB3	2.11	0.66
2:B:151:PRO:O	2:B:212:HIS:HD2	1.79	0.66
1:C:115:VAL:HG22	1:C:136:LEU:HG	1.77	0.65
1:C:37:LEU:HD13	1:C:86:TYR:CE1	2.32	0.65
1:C:108:ARG:NH2	1:C:111:ALA:HB2	2.12	0.65
1:C:160:LEU:HD11	2:D:177:VAL:HB	1.79	0.65
1:C:11:LEU:HD23	1:C:104:LEU:HD23	1.79	0.64
2:D:27:TYR:HB2	2:D:94:ARG:HH12	1.62	0.64
1:C:14:SER:O	1:C:17:ASP:HB2	1.97	0.64
1:A:48:ILE:HD12	1:A:73:LEU:HD23	1.80	0.64
1:A:124:GLN:HG2	1:A:129:GLY:O	1.97	0.64
1:A:190:ASN:O	1:A:210:ASN:HA	1.98	0.64
2:D:35:HIS:HD2	2:D:47:TRP:NE1	1.94	0.64
1:A:198:HIS:CD2	1:A:199:LYS:H	2.16	0.64
2:B:48:ILE:HD13	2:B:80:MET:HE1	1.80	0.64
1:C:38:GLN:HE22	2:D:39:GLN:HE22	1.44	0.64
1:C:42:GLN:OE1	1:C:45:LYS:HE3	1.98	0.64
2:D:29:PHE:CE2	2:D:52(A):PRO:HB3	2.33	0.64
2:B:87:SER:HB3	2:B:111:VAL:H	1.64	0.63
2:B:178:LEU:HD13	2:B:183:ASP:HA	1.79	0.63
2:D:154:LEU:HA	2:D:209:ASN:O	1.99	0.63
2:B:127:GLY:CA	2:D:131:GLN:HB2	2.21	0.62
1:A:67:SER:O	1:A:69:THR:N	2.32	0.62
1:A:161:ASN:HA	1:A:176:SER:O	1.98	0.62
1:C:133:VAL:HG22	1:C:178:THR:HG23	1.82	0.62
1:C:135:PHE:CD2	2:D:190:SER:HB3	2.34	0.62
1:A:24:ARG:HH21	1:A:70:ASP:CG	2.07	0.62
2:B:13:LYS:HZ1	2:B:113:SER:HA	1.65	0.62
2:B:35:HIS:HD2	2:B:47:TRP:NE1	1.96	0.62
1:A:76:SER:O	1:A:77:ARG:HB2	2.00	0.62
2:B:131:GLN:HG2	2:D:130:ALA:HA	1.82	0.62
1:C:117:ILE:H	1:C:207:LYS:HE2	1.63	0.61
2:D:166:LEU:HD12	2:D:166:LEU:N	2.14	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:144:ILE:HD12	1:A:198:HIS:ND1	2.15	0.61
2:D:24:ALA:HB3	2:D:29:PHE:HD1	1.65	0.61
1:C:136:LEU:HD21	1:C:146:VAL:HG22	1.82	0.61
1:C:27(D):HIS:CD2	1:C:28:ASN:H	2.17	0.61
2:D:12:VAL:O	2:D:111:VAL:HA	2.00	0.61
2:D:198:PRO:O	2:D:202:SER:HB3	2.00	0.61
2:B:59:TYR:CE2	2:B:69:LEU:HG	2.35	0.61
2:B:178:LEU:O	2:B:178:LEU:HD12	2.00	0.61
1:C:183:LYS:O	1:C:187:GLU:HG2	2.00	0.60
2:D:35:HIS:CD2	2:D:47:TRP:HE1	2.06	0.60
2:B:30:THR:HG22	2:B:52(A):PRO:O	2.01	0.60
2:B:89:VAL:HG21	4:B:259:HOH:O	1.99	0.60
2:D:9:PRO:HB3	4:D:361:HOH:O	2.01	0.60
1:A:150:ILE:HG13	1:A:155:ARG:NE	2.16	0.59
2:B:13:LYS:NZ	2:B:113:SER:HA	2.16	0.59
2:D:132:THR:HB	2:D:137:MET:O	2.02	0.59
2:B:39:GLN:CB	2:B:91:TYR:HE1	2.15	0.59
1:C:12:PRO:HA	1:C:105:GLU:O	2.02	0.59
1:A:7:THR:HG23	4:A:298:HOH:O	2.02	0.59
1:A:83:LEU:HD23	1:A:104:LEU:O	2.01	0.59
1:A:29:GLY:O	1:A:30:ASN:ND2	2.36	0.59
1:A:139:PHE:CE2	1:A:144:ILE:HG21	2.38	0.59
2:B:123:PRO:HG2	2:B:223:ILE:HD13	1.85	0.59
2:B:154:LEU:HD23	2:B:189:SER:HB3	1.84	0.59
2:B:194:THR:HB	2:B:198:PRO:CD	2.33	0.59
2:D:137:MET:HA	2:D:193:VAL:O	2.02	0.59
1:A:209:PHE:CB	2:B:128:SER:HB3	2.28	0.58
1:C:158:GLY:O	1:C:179:LEU:HA	2.03	0.58
1:A:35:TRP:HB2	1:A:48:ILE:HB	1.85	0.58
2:B:12:VAL:CG1	2:B:16:ALA:HB3	2.32	0.58
2:D:213:PRO:HG2	2:D:214:ALA:H	1.69	0.58
1:C:135:PHE:C	1:C:136:LEU:HD12	2.27	0.58
1:C:189:HIS:HB2	1:C:192:TYR:OH	2.03	0.58
2:D:27:TYR:HB2	2:D:94:ARG:NH1	2.18	0.58
2:B:12:VAL:HG12	2:B:16:ALA:HB3	1.85	0.58
2:B:162:ASN:O	2:B:165:SER:HB2	2.03	0.58
1:A:90:GLN:HE21	1:A:97:THR:H	1.52	0.58
2:B:69:LEU:HD21	2:B:80:MET:HG3	1.85	0.58
2:D:9:PRO:O	2:D:9:PRO:HG2	2.04	0.58
2:B:72:ASP:HB2	2:B:79:TYR:HE1	1.69	0.57
1:A:86:TYR:CE2	1:A:104:LEU:HG	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:209:PHE:HB3	2:B:128:SER:CB	2.28	0.57
1:C:4:MET:HA	1:C:4:MET:HE3	1.86	0.57
1:C:207:LYS:HG3	1:C:208:SER:N	2.20	0.57
2:D:157:TRP:HA	2:D:206:THR:O	2.04	0.57
1:C:5:THR:CG2	1:C:24:ARG:HD3	2.32	0.57
2:B:11:LEU:CD2	2:B:149:PRO:HG3	2.25	0.57
2:B:178:LEU:HB3	2:B:185:TYR:CE1	2.39	0.57
1:A:91:GLY:HA3	3:B:227:1PC:HL1	1.86	0.57
1:A:162:SER:OG	2:B:175:PRO:HG2	2.04	0.57
1:C:139:PHE:O	1:C:172:THR:HB	2.05	0.56
1:C:174:SER:OG	2:D:172:HIS:HD2	1.87	0.56
2:D:105:GLN:H	2:D:105:GLN:NE2	2.03	0.56
1:A:34:GLU:O	1:A:88:CYS:HA	2.05	0.56
2:B:14:PRO:HA	2:B:82(C):LEU:O	2.04	0.56
2:D:115:LYS:HG2	4:D:394:HOH:O	2.04	0.56
1:A:39:LYS:HB2	1:A:42:GLN:HG3	1.86	0.56
2:D:154:LEU:HD11	2:D:189:SER:HB2	1.88	0.56
1:C:1:ASP:OD1	1:C:1:ASP:N	2.36	0.56
2:D:24:ALA:HB3	2:D:29:PHE:CD1	2.40	0.56
1:A:113:PRO:HG3	1:A:144:ILE:HD11	1.87	0.56
2:B:154:LEU:HD12	2:B:156:THR:H	1.71	0.56
2:D:52(A):PRO:HA	2:D:71:VAL:HG21	1.87	0.56
2:B:119:PRO:HB2	2:B:144:VAL:HG12	1.86	0.56
2:B:178:LEU:HA	2:B:184:LEU:O	2.05	0.56
2:B:47:TRP:CH2	2:B:49:GLY:HA2	2.42	0.55
2:B:209:ASN:N	2:B:209:ASN:ND2	2.52	0.55
2:D:11:LEU:HD11	2:D:112:SER:OG	2.06	0.55
1:A:38:GLN:HE22	2:B:39:GLN:HE21	1.54	0.55
1:C:164:THR:HG22	1:C:174:SER:H	1.72	0.55
1:A:140:TYR:CE1	1:A:141:PRO:HA	2.42	0.55
2:B:137:MET:O	2:B:137:MET:SD	2.64	0.55
2:D:38:LYS:O	2:D:45:LEU:HD23	2.06	0.55
2:D:34:ILE:HD13	2:D:78:ALA:HB2	1.89	0.55
2:D:203:GLU:HB2	4:D:267:HOH:O	2.05	0.55
2:B:127:GLY:HA2	2:D:131:GLN:H	1.70	0.55
2:D:162:ASN:HD21	2:D:205:VAL:HA	1.71	0.55
2:D:168:SER:C	2:D:171:VAL:H	2.15	0.55
2:B:96:THR:HG22	2:B:98:ASP:H	1.72	0.54
1:C:11:LEU:HD21	1:C:19:ALA:HB1	1.88	0.54
2:B:119:PRO:HB2	2:B:144:VAL:CG1	2.37	0.54
1:C:27(D):HIS:HD2	1:C:28:ASN:N	2.03	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:9:LEU:HD23	1:C:9:LEU:H	1.72	0.54
1:C:4:MET:HA	1:C:4:MET:HE2	1.89	0.54
2:B:20:MET:HE1	2:B:90:TYR:HB2	1.89	0.54
1:A:16:GLY:C	1:A:77:ARG:HA	2.33	0.54
1:C:68:GLY:O	1:C:71:PHE:CZ	2.61	0.54
1:C:27(C):VAL:HG21	4:C:262:HOH:O	2.07	0.54
1:A:155:ARG:HD2	1:A:179:LEU:HD11	1.89	0.53
2:B:59:TYR:HE2	2:B:69:LEU:HG	1.73	0.53
1:C:54:ARG:HD3	1:C:58:VAL:HG12	1.91	0.53
1:C:135:PHE:CE2	2:D:190:SER:HB3	2.43	0.53
2:D:149:PRO:HD2	2:D:214:ALA:CB	2.37	0.53
2:B:24:ALA:HB3	2:B:29:PHE:HD1	1.72	0.53
2:B:48:ILE:HD13	2:B:80:MET:CE	2.37	0.53
3:C:212:1PC:HR2	2:D:97:TRP:O	2.08	0.53
2:B:28:THR:HG22	2:B:31:ASP:H	1.72	0.53
1:A:143:ASP:HB2	1:A:199:LYS:HE2	1.90	0.53
1:A:149:LYS:HG2	1:A:154:GLU:HA	1.90	0.53
1:A:161:ASN:ND2	1:A:177:SER:OG	2.42	0.53
1:A:187:GLU:HA	1:A:211:ARG:HH21	1.72	0.53
2:B:196:SER:O	2:B:202:SER:HB3	2.09	0.53
1:A:108:ARG:HD2	1:A:171:SER:CB	2.37	0.53
1:C:6:GLN:NE2	1:C:35:TRP:CZ3	2.77	0.53
1:C:6:GLN:HE22	1:C:35:TRP:HZ3	1.57	0.53
2:D:12:VAL:HG12	2:D:16:ALA:HB3	1.91	0.53
2:D:123:PRO:HG3	2:D:221:LYS:HG3	1.90	0.53
2:D:166:LEU:H	2:D:166:LEU:CD1	2.20	0.53
2:D:219:VAL:HG11	4:D:342:HOH:O	2.08	0.53
1:A:204:PRO:O	1:C:190:ASN:ND2	2.42	0.53
2:D:65:GLY:O	2:D:82(A):ARG:NH2	2.42	0.52
2:D:166:LEU:HD23	2:D:193:VAL:HG11	1.90	0.52
2:B:223:ILE:HG13	2:B:226:VAL:H	1.74	0.52
1:A:27(A):THR:HG22	1:A:27(C):VAL:H	1.74	0.52
1:A:33:LEU:HA	1:A:89:PHE:O	2.09	0.52
2:B:2:VAL:HB	2:B:102:TYR:CD2	2.44	0.52
1:C:164:THR:HG23	1:C:165:ASP:O	2.10	0.52
1:A:13:VAL:HG21	1:A:78:VAL:HG21	1.92	0.52
2:B:213:PRO:O	2:B:215:SER:N	2.42	0.52
1:C:166:GLN:HA	1:C:172:THR:O	2.10	0.52
2:D:29:PHE:CE1	2:D:34:ILE:HD11	2.44	0.52
2:D:166:LEU:HD23	2:D:193:VAL:CG1	2.39	0.52
1:C:110:ASP:OD2	1:C:200:THR:HG23	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:135:PHE:CE2	2:B:190:SER:HB3	2.45	0.52
2:B:89:VAL:HA	2:B:107:THR:O	2.08	0.52
1:C:136:LEU:HD21	1:C:146:VAL:HG23	1.92	0.52
2:B:14:PRO:C	2:B:16:ALA:H	2.18	0.52
1:A:96:TYR:CE2	3:B:227:IPC:HF	2.45	0.51
2:D:6:GLN:OE1	2:D:91:TYR:HA	2.10	0.51
1:C:2:VAL:HG21	1:C:93:HIS:ND1	2.24	0.51
1:A:18:GLN:HG2	1:A:76:SER:HA	1.92	0.51
1:A:144:ILE:HD12	1:A:198:HIS:CG	2.45	0.51
2:B:145:LYS:HB2	2:B:186:THR:HG23	1.91	0.51
1:C:140:TYR:HB2	1:C:172:THR:HG22	1.90	0.51
2:D:194:THR:O	2:D:198:PRO:HD2	2.10	0.51
2:B:123:PRO:CG	2:B:223:ILE:HD13	2.41	0.51
2:B:149:PRO:HD2	2:B:214:ALA:HB3	1.93	0.51
1:A:2:VAL:HG12	1:A:27:GLN:HG2	1.93	0.51
1:C:117:ILE:HG12	1:C:134:CYS:HB2	1.93	0.51
1:A:37:LEU:HB2	1:A:47:LEU:HD11	1.93	0.51
2:D:27:TYR:CB	2:D:94:ARG:NH1	2.73	0.51
1:A:15:LEU:HD12	1:A:108:ARG:HH21	1.76	0.50
1:A:61:ARG:NH2	1:A:81:GLU:OE2	2.44	0.50
1:A:59:PRO:HG2	1:A:62:PHE:CD2	2.46	0.50
1:A:113:PRO:HG3	1:A:144:ILE:CD1	2.41	0.50
1:C:142:LYS:HB2	1:C:173:TYR:CZ	2.45	0.50
1:C:49:TYR:O	1:C:53:ASN:HB2	2.11	0.50
2:D:93:GLY:HA2	2:D:103:TRP:HA	1.93	0.50
2:D:121:VAL:O	2:D:221:LYS:HE2	2.12	0.50
2:D:187:LEU:C	2:D:187:LEU:HD23	2.37	0.50
2:B:152:VAL:HG23	2:B:212:HIS:CD2	2.47	0.49
2:B:29:PHE:CE2	2:B:52(A):PRO:HB3	2.47	0.49
2:D:157:TRP:O	2:D:162:ASN:C	2.55	0.49
2:B:223:ILE:HG23	2:B:226:VAL:H	1.74	0.49
2:D:137:MET:SD	2:D:193:VAL:C	2.95	0.49
2:B:87:SER:HA	2:B:109:LEU:O	2.12	0.49
1:C:40:PRO:HB2	4:C:357:HOH:O	2.10	0.49
2:D:132:THR:O	2:D:133:ASN:C	2.55	0.49
1:A:2:VAL:HG23	1:A:90:GLN:NE2	2.28	0.49
1:A:34:GLU:HB2	1:A:89:PHE:HB3	1.93	0.49
1:A:42:GLN:HB3	4:A:347:HOH:O	2.12	0.49
1:C:161:ASN:HB3	1:C:163:TRP:CZ3	2.48	0.49
1:A:117:ILE:H	2:B:129:ALA:HB2	1.77	0.49
2:B:174:PHE:CD1	2:B:174:PHE:N	2.81	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:90:GLN:NE2	1:A:97:THR:H	2.11	0.49
2:B:40:SER:O	2:B:41:HIS:HB2	2.13	0.49
2:B:206:THR:HA	2:B:221:LYS:O	2.13	0.49
1:A:130:ALA:HB3	1:A:181:LEU:O	2.13	0.48
2:B:140:LEU:HD11	2:B:199:ARG:HG3	1.94	0.48
1:C:193:THR:CG2	1:C:206:VAL:HG13	2.43	0.48
1:C:86:TYR:HE2	1:C:104:LEU:HG	1.77	0.48
1:A:59:PRO:HG2	1:A:62:PHE:CE2	2.48	0.48
2:B:119:PRO:CA	2:B:147:TYR:HB3	2.43	0.48
2:D:39:GLN:O	2:D:88:ALA:HB1	2.13	0.48
2:B:118:PRO:HB3	2:B:217:THR:HG21	1.94	0.48
1:C:12:PRO:HA	1:C:105:GLU:HG3	1.95	0.48
1:C:62:PHE:CE1	1:C:75:ILE:HG12	2.47	0.48
1:C:174:SER:OG	2:D:172:HIS:CD2	2.66	0.48
2:B:119:PRO:HB3	2:B:147:TYR:HB3	1.95	0.48
1:C:150:ILE:HD12	1:C:150:ILE:N	2.28	0.48
1:A:121:SER:O	1:A:125:LEU:HD22	2.13	0.48
1:A:190:ASN:HB2	1:C:203:SER:CB	2.21	0.48
1:C:27(C):VAL:CA	1:C:31:THR:HG23	2.42	0.48
2:D:27:TYR:CG	2:D:94:ARG:NH1	2.81	0.48
1:A:90:GLN:O	1:A:90:GLN:CD	2.56	0.48
1:A:91:GLY:HA2	1:A:96:TYR:CD1	2.49	0.48
2:B:174:PHE:HD1	2:B:188:SER:O	1.97	0.48
1:A:8:PRO:HG3	1:A:11:LEU:CD1	2.26	0.47
2:B:115:LYS:H	2:B:115:LYS:CD	2.18	0.47
1:C:12:PRO:CA	1:C:105:GLU:HG3	2.44	0.47
2:D:154:LEU:HD23	2:D:154:LEU:N	2.27	0.47
2:B:24:ALA:HB1	2:B:27:TYR:CE1	2.49	0.47
1:C:91:GLY:O	3:C:212:1PC:HN2	2.14	0.47
2:B:6:GLN:HB2	2:B:22:CYS:SG	2.54	0.47
2:B:66:LYS:CE	2:B:82:VAL:HG13	2.45	0.47
2:B:121:VAL:CG2	2:B:210:VAL:HG21	2.44	0.47
1:A:24:ARG:NH2	1:A:70:ASP:OD2	2.45	0.47
1:A:166:GLN:HA	1:A:172:THR:O	2.14	0.47
1:A:83:LEU:HD11	1:A:166:GLN:HG2	1.96	0.47
1:A:89:PHE:CE1	1:A:96:TYR:HB3	2.49	0.47
2:B:11:LEU:H	2:B:11:LEU:HD23	1.80	0.47
2:B:97:TRP:O	3:B:227:1PC:CR	2.56	0.47
2:B:209:ASN:N	2:B:209:ASN:HD22	2.11	0.47
1:C:34:GLU:O	1:C:88:CYS:HA	2.15	0.47
1:C:62:PHE:CD1	1:C:75:ILE:HG12	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:24:ALA:CB	2:D:29:PHE:HD1	2.28	0.47
2:D:69:LEU:CD2	2:D:80:MET:HG3	2.44	0.47
1:A:175:MET:CG	1:A:176:SER:N	2.77	0.47
2:D:205:VAL:O	2:D:223:ILE:HG12	2.15	0.47
1:A:2:VAL:CG2	1:A:90:GLN:NE2	2.78	0.47
2:B:21:SER:HB2	2:B:77:THR:CG2	2.44	0.47
2:B:66:LYS:HZ3	2:B:82:VAL:HG13	1.76	0.47
2:B:35:HIS:CE1	2:B:95:SER:OG	2.68	0.46
1:C:150:ILE:HD13	1:C:155:ARG:CB	2.45	0.46
2:D:30:THR:HA	2:D:52(A):PRO:HB2	1.96	0.46
1:A:188:ARG:O	1:A:188:ARG:HG3	2.15	0.46
2:B:39:GLN:HB2	2:B:91:TYR:HE1	1.80	0.46
1:A:121:SER:HB3	2:B:123:PRO:O	2.15	0.46
1:A:160:LEU:HD23	2:B:177:VAL:CG1	2.45	0.46
2:B:5:GLN:OE1	2:B:23:LYS:HG2	2.15	0.46
1:A:16:GLY:HA2	1:A:77:ARG:HG2	1.96	0.46
1:A:116:SER:O	1:A:134:CYS:HA	2.16	0.46
1:A:187:GLU:O	1:A:211:ARG:NH2	2.48	0.46
2:B:61:HIS:HB2	4:B:334:HOH:O	2.14	0.46
2:B:196:SER:HB2	2:B:198:PRO:CD	2.42	0.46
1:C:58:VAL:HA	1:C:59:PRO:HD3	1.76	0.46
1:C:144:ILE:HG23	1:C:175:MET:CE	2.46	0.46
2:D:150:GLU:O	2:D:150:GLU:HG2	2.16	0.46
1:A:150:ILE:CD1	1:A:179:LEU:HD21	2.41	0.46
1:C:202:THR:HG22	1:C:202:THR:O	2.15	0.46
2:B:115:LYS:HB3	2:B:115:LYS:HZ2	1.81	0.46
2:B:127:GLY:HA2	2:D:131:GLN:N	2.31	0.46
2:B:151:PRO:O	2:B:212:HIS:CD2	2.64	0.46
2:D:52:TYR:O	2:D:53:ASN:N	2.49	0.46
1:A:6:GLN:HG2	1:A:102:THR:OG1	2.15	0.46
2:D:166:LEU:CD2	2:D:193:VAL:HG11	2.47	0.46
2:B:47:TRP:CZ2	2:B:49:GLY:HA2	2.51	0.45
2:B:115:LYS:HB3	2:B:115:LYS:HZ3	1.81	0.45
2:D:212:HIS:ND1	2:D:215:SER:OG	2.46	0.45
1:C:136:LEU:O	1:C:139:PHE:HE1	1.99	0.45
2:B:20:MET:HE2	2:B:36:TRP:CZ3	2.52	0.45
2:B:121:VAL:HG21	2:B:210:VAL:HG21	1.98	0.45
1:C:31:THR:HB	1:C:51:VAL:HG21	1.98	0.45
1:C:37:LEU:HB2	1:C:47:LEU:HD11	1.98	0.45
1:C:83:LEU:HA	1:C:104:LEU:HD12	1.97	0.45
1:C:117:ILE:HG23	1:C:118:PHE:N	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:38:GLN:HE22	2:B:39:GLN:NE2	2.14	0.45
1:C:120:PRO:HD3	1:C:132:VAL:HG22	1.97	0.45
2:D:33:TYR:N	2:D:33:TYR:CD1	2.85	0.45
2:D:194:THR:HB	2:D:198:PRO:CD	2.47	0.45
1:C:207:LYS:CE	2:D:129:ALA:HB2	2.46	0.45
1:A:14:SER:O	1:A:17:ASP:HB2	2.17	0.45
1:A:118:PHE:CE1	1:A:135:PHE:CD2	3.05	0.45
1:C:130:ALA:HB3	1:C:181:LEU:HD23	1.98	0.45
1:A:48:ILE:HD13	1:A:64:GLY:HA3	1.98	0.45
1:C:13:VAL:HG21	1:C:78:VAL:HG21	1.99	0.45
2:D:151:PRO:O	2:D:213:PRO:HD2	2.17	0.45
2:B:223:ILE:HD12	2:B:223:ILE:HA	1.81	0.44
2:D:200:PRO:O	2:D:202:SER:C	2.60	0.44
1:A:111:ALA:O	1:A:200:THR:HG21	2.17	0.44
1:A:156:GLN:O	1:A:159:VAL:HG23	2.16	0.44
2:B:48:ILE:HG12	2:B:63:PHE:CD2	2.52	0.44
2:B:54:ASN:OD1	2:B:56:GLY:N	2.46	0.44
1:C:175:MET:N	2:D:174:PHE:HE2	2.15	0.44
1:A:49:TYR:CD1	1:A:49:TYR:O	2.71	0.44
1:C:31:THR:HB	1:C:51:VAL:CG2	2.48	0.44
1:C:113:PRO:HA	1:C:137:ASN:O	2.17	0.44
1:C:138:ASN:HA	1:C:173:TYR:O	2.16	0.44
1:C:184:ASP:HB3	1:C:188:ARG:HH21	1.71	0.44
1:A:89:PHE:CE2	2:B:100:PHE:HE2	2.36	0.44
1:A:135:PHE:CD2	2:B:190:SER:HB3	2.53	0.44
2:B:154:LEU:HD12	2:B:154:LEU:C	2.41	0.44
1:A:182:THR:O	1:A:185:GLU:N	2.51	0.44
2:B:97:TRP:O	3:B:227:1PC:HB	2.17	0.44
2:B:162:ASN:HB2	2:B:166:LEU:HG	2.00	0.44
2:B:208:CYS:C	2:B:209:ASN:HD22	2.26	0.44
2:D:157:TRP:CE3	2:D:205:VAL:HG12	2.53	0.44
1:C:27(D):HIS:CD2	1:C:27(E):SER:N	2.85	0.44
1:C:136:LEU:CD2	1:C:146:VAL:CG2	2.93	0.44
2:D:148:PHE:CD1	2:D:148:PHE:C	2.96	0.44
2:D:70:THR:HG23	2:D:79:TYR:HB2	1.99	0.43
1:A:89:PHE:CE2	2:B:100:PHE:CE2	3.06	0.43
1:C:108:ARG:HB3	4:C:295:HOH:O	2.17	0.43
2:D:123:PRO:HG3	2:D:221:LYS:CG	2.48	0.43
2:D:196:SER:N	2:D:198:PRO:CD	2.81	0.43
1:C:12:PRO:HB3	1:C:105:GLU:HG3	2.01	0.43
1:A:86:TYR:O	1:A:101:GLY:HA2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:146:GLY:HA2	2:B:184:LEU:HB3	2.00	0.43
1:C:62:PHE:HE1	1:C:75:ILE:CD1	2.30	0.43
2:B:42:GLY:HA2	4:B:259:HOH:O	2.17	0.43
2:D:89:VAL:HA	2:D:107:THR:O	2.18	0.43
1:A:37:LEU:HD13	1:A:86:TYR:CZ	2.54	0.43
1:A:189:HIS:HB2	1:A:192:TYR:OH	2.17	0.43
1:A:193:THR:CG2	1:A:206:VAL:HG13	2.48	0.43
2:B:38:LYS:HD2	2:B:63:PHE:HE2	1.83	0.43
3:C:212:1PC:HR1	2:D:97:TRP:O	2.17	0.43
2:D:152:VAL:HG23	2:D:211:ALA:O	2.19	0.43
1:A:155:ARG:HG2	4:A:339:HOH:O	2.19	0.43
1:C:139:PHE:HZ	1:C:175:MET:HB3	1.83	0.43
1:A:38:GLN:HB2	1:A:44:PRO:HG3	2.00	0.43
2:B:147:TYR:CE1	2:B:185:TYR:HB2	2.53	0.43
1:A:13:VAL:O	1:A:107:LYS:N	2.51	0.43
1:A:124:GLN:NE2	1:A:131:SER:H	2.17	0.42
2:B:3:GLN:H	2:B:3:GLN:HG2	1.70	0.42
2:B:22:CYS:O	2:B:77:THR:HA	2.18	0.42
2:B:102:TYR:CD1	2:B:102:TYR:N	2.87	0.42
2:B:154:LEU:CD2	2:B:189:SER:HB3	2.48	0.42
1:A:198:HIS:HD2	1:A:199:LYS:H	1.66	0.42
1:C:144:ILE:HG12	1:C:145:ASN:N	2.33	0.42
2:D:23:LYS:NZ	4:D:371:HOH:O	2.45	0.42
2:B:215:SER:HB2	2:B:217:THR:HG1	1.83	0.42
2:B:35:HIS:HE1	2:B:95:SER:OG	2.02	0.42
2:B:156:THR:CG2	2:B:157:TRP:N	2.82	0.42
1:C:9:LEU:H	1:C:9:LEU:CD2	2.30	0.42
1:C:112:ALA:HB1	1:C:205:ILE:HD11	2.01	0.42
2:B:61:HIS:ND1	2:B:61:HIS:N	2.66	0.42
2:B:115:LYS:HD2	2:B:115:LYS:N	2.28	0.42
2:B:199:ARG:HH11	2:B:199:ARG:CB	2.24	0.42
2:D:214:ALA:HA	4:D:348:HOH:O	2.19	0.42
2:B:1:GLU:O	2:B:3:GLN:N	2.52	0.42
2:B:2:VAL:HG21	2:B:94:ARG:HH22	1.82	0.42
1:C:27(A):THR:O	1:C:93:HIS:HE1	2.02	0.42
1:A:124:GLN:HE22	1:A:131:SER:HB2	1.83	0.42
1:A:189:HIS:O	1:A:211:ARG:CD	2.67	0.42
1:A:198:HIS:CE1	1:A:200:THR:HG23	2.55	0.42
2:B:148:PHE:O	2:B:212:HIS:HE1	2.02	0.42
2:B:171:VAL:HG22	4:B:380:HOH:O	2.19	0.42
1:C:139:PHE:CE2	1:C:144:ILE:HG21	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:60:ASN:ND2	2:D:62:LYS:HG3	2.34	0.42
1:A:27(D):HIS:CD2	1:A:27(E):SER:H	2.38	0.41
1:A:203:SER:OG	1:C:190:ASN:HB3	2.20	0.41
1:C:76:SER:O	1:C:77:ARG:CB	2.68	0.41
1:C:150:ILE:HD13	1:C:155:ARG:HB3	2.02	0.41
2:D:157:TRP:CH2	2:D:208:CYS:HB3	2.55	0.41
1:A:3:LEU:HD12	1:A:3:LEU:HA	1.90	0.41
1:A:150:ILE:O	1:A:153:SER:OG	2.37	0.41
1:A:182:THR:C	1:A:184:ASP:N	2.77	0.41
2:B:52(A):PRO:O	2:B:73:LYS:HD3	2.21	0.41
1:C:36:TYR:HA	1:C:45:LYS:O	2.21	0.41
1:A:80:ALA:C	1:A:82:ASP:H	2.27	0.41
1:C:51:VAL:HG12	1:C:52:THR:HG23	2.03	0.41
1:C:80:ALA:CB	1:C:168:SER:O	2.66	0.41
1:A:209:PHE:HB2	2:B:128:SER:OG	2.21	0.41
2:B:29:PHE:HE2	2:B:71:VAL:HG13	1.86	0.41
1:A:36:TYR:HB2	1:A:87:TYR:HB2	2.03	0.41
2:B:36:TRP:HD1	2:B:69:LEU:HD13	1.85	0.41
2:D:33:TYR:N	2:D:33:TYR:HD1	2.19	0.41
1:A:209:PHE:CB	2:B:128:SER:CB	2.93	0.41
1:A:4:MET:HE3	1:A:90:GLN:HG2	2.02	0.41
2:B:86:ASP:HB2	2:B:111:VAL:HG21	2.03	0.41
1:A:115:VAL:HG22	1:A:136:LEU:HD23	2.03	0.41
2:B:12:VAL:HG12	2:B:13:LYS:O	2.20	0.41
2:B:180:SER:O	2:B:183:ASP:HB2	2.21	0.41
1:C:61:ARG:HD2	1:C:75:ILE:CG2	2.50	0.41
1:A:27(E):SER:C	1:A:29:GLY:H	2.28	0.41
1:A:192:TYR:HB2	1:A:209:PHE:CE2	2.56	0.41
2:B:39:GLN:HB3	2:B:91:TYR:HE1	1.84	0.41
2:B:206:THR:HG21	4:B:237:HOH:O	2.20	0.41
1:C:147:LYS:O	1:C:194:CYS:HA	2.19	0.41
1:C:193:THR:HG23	1:C:206:VAL:HG13	2.03	0.41
2:D:43:LYS:HD3	4:D:329:HOH:O	2.21	0.41
2:D:168:SER:HA	4:D:391:HOH:O	2.19	0.41
2:D:174:PHE:HA	2:D:175:PRO:HD3	1.86	0.41
1:A:120:PRO:HD2	1:A:186:TYR:OH	2.20	0.41
2:B:52(A):PRO:HG3	2:B:71:VAL:HG21	2.03	0.41
1:A:33:LEU:HD22	1:A:71:PHE:CD2	2.56	0.40
1:A:32:TYR:O	1:A:90:GLN:HA	2.22	0.40
2:B:184:LEU:CD2	2:B:184:LEU:N	2.85	0.40
1:C:116:SER:O	1:C:134:CYS:HA	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:139:PHE:CD1	1:C:139:PHE:N	2.89	0.40
2:D:105:GLN:CD	2:D:105:GLN:N	2.71	0.40
1:A:27(E):SER:C	1:A:29:GLY:N	2.80	0.40
2:B:13:LYS:HE3	2:B:13:LYS:HB3	1.86	0.40
2:B:171:VAL:HG12	2:B:191:VAL:CG2	2.46	0.40
2:D:156:THR:O	2:D:208:CYS:HA	2.21	0.40
1:A:37:LEU:CD2	4:A:344:HOH:O	2.69	0.40
2:B:20:MET:CE	2:B:107:THR:HG21	2.52	0.40
2:B:132:THR:HG23	2:B:138:VAL:HG21	2.03	0.40
2:D:96:THR:HG23	2:D:98:ASP:H	1.86	0.40
2:B:66:LYS:HE2	2:B:82:VAL:CG1	2.51	0.40
1:C:91:GLY:O	3:C:212:IPC:CN	2.70	0.40
1:C:115:VAL:HA	1:C:135:PHE:O	2.21	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	214/216 (99%)	193 (90%)	19 (9%)	2 (1%)	14	14
1	C	214/216 (99%)	190 (89%)	21 (10%)	3 (1%)	9	7
2	B	213/215 (99%)	181 (85%)	20 (9%)	12 (6%)	1	0
2	D	213/215 (99%)	181 (85%)	26 (12%)	6 (3%)	4	2
All	All	854/862 (99%)	745 (87%)	86 (10%)	23 (3%)	4	2

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	68	GLY
2	B	131	GLN

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Mol	Chain	Res	Type
2	B	198	PRO
2	B	214	ALA
1	C	68	GLY
2	B	2	VAL
2	B	126	PRO
2	B	223	ILE
1	C	202	THR
2	D	133	ASN
2	B	82(C)	LEU
2	D	52(A)	PRO
2	B	118	PRO
2	B	130	ALA
2	B	150	GLU
2	D	198	PRO
1	C	143	ASP
2	D	64	LYS
2	D	146	GLY
2	D	202	SER
2	B	8	GLY
1	A	144	ILE
2	B	52(A)	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	192/192 (100%)	168 (88%)	24 (12%)	4	4
1	C	192/192 (100%)	155 (81%)	37 (19%)	1	1
2	B	186/186 (100%)	138 (74%)	48 (26%)	0	0
2	D	186/186 (100%)	151 (81%)	35 (19%)	1	1
All	All	756/756 (100%)	612 (81%)	144 (19%)	1	1

All (144) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	VAL
1	A	5	THR
1	A	9	LEU
1	A	10	SER
1	A	56	SER
1	A	65	SER
1	A	73	LEU
1	A	83	LEU
1	A	92	THR
1	A	97	THR
1	A	103	LYS
1	A	104	LEU
1	A	121	SER
1	A	123	GLU
1	A	125	LEU
1	A	127	SER
1	A	132	VAL
1	A	133	VAL
1	A	144	ILE
1	A	164	THR
1	A	180	THR
1	A	181	LEU
1	A	210	ASN
1	A	211	ARG
2	B	3	GLN
2	B	19	LYS
2	B	20	MET
2	B	22	CYS
2	B	28	THR
2	B	40	SER
2	B	41	HIS
2	B	44	SER
2	B	51	ILE
2	B	61	HIS
2	B	62	LYS
2	B	66	LYS
2	B	68	THR
2	B	70	THR
2	B	71	VAL
2	B	75	SER
2	B	82	VAL
2	B	82(A)	ARG
2	B	82(B)	THR

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Mol	Chain	Res	Type
2	B	82(C)	LEU
2	B	92	CYS
2	B	96	THR
2	B	101	ASP
2	B	105	GLN
2	B	107	THR
2	B	113	SER
2	B	115	LYS
2	B	117	THR
2	B	119	PRO
2	B	137	MET
2	B	152	VAL
2	B	154	LEU
2	B	156	THR
2	B	165	SER
2	B	171	VAL
2	B	184	LEU
2	B	187	LEU
2	B	188	SER
2	B	193	VAL
2	B	195	SER
2	B	198	PRO
2	B	199	ARG
2	B	204	THR
2	B	209	ASN
2	B	213	PRO
2	B	217	THR
2	B	219	VAL
2	B	223	ILE
1	C	1	ASP
1	C	3	LEU
1	C	4	MET
1	C	5	THR
1	C	9	LEU
1	C	10	SER
1	C	14	SER
1	C	15	LEU
1	C	17	ASP
1	C	26	SER
1	C	31	THR
1	C	33	LEU
1	C	39	LYS

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Mol	Chain	Res	Type
1	C	50	LYS
1	C	77	ARG
1	C	83	LEU
1	C	92	THR
1	C	103	LYS
1	C	104	LEU
1	C	117	ILE
1	C	122	SER
1	C	123	GLU
1	C	125	LEU
1	C	126	THR
1	C	131	SER
1	C	144	ILE
1	C	153	SER
1	C	154	GLU
1	C	157	ASN
1	C	160	LEU
1	C	167	ASP
1	C	168	SER
1	C	175	MET
1	C	181	LEU
1	C	182	THR
1	C	198	HIS
1	C	202	THR
2	D	2	VAL
2	D	5	GLN
2	D	19	LYS
2	D	25	SER
2	D	33	TYR
2	D	41	HIS
2	D	54	ASN
2	D	57	ASN
2	D	70	THR
2	D	74	SER
2	D	77	THR
2	D	82	VAL
2	D	82(A)	ARG
2	D	82(B)	THR
2	D	82(C)	LEU
2	D	85	GLU
2	D	96	THR
2	D	101	ASP

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Mol	Chain	Res	Type
2	D	105	GLN
2	D	109	LEU
2	D	110	THR
2	D	116	THR
2	D	136	SER
2	D	140	LEU
2	D	156	THR
2	D	167	SER
2	D	186	THR
2	D	187	LEU
2	D	194	THR
2	D	195	SER
2	D	196	SER
2	D	198	PRO
2	D	199	ARG
2	D	204	THR
2	D	210	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	157	ASN
1	A	161	ASN
1	A	190	ASN
1	A	198	HIS
2	B	35	HIS
2	B	39	GLN
2	B	41	HIS
2	B	131	GLN
2	B	212	HIS
1	C	27	GLN
1	C	27(D)	HIS
1	C	30	ASN
1	C	53	ASN
1	C	156	GLN
1	C	157	ASN
1	C	166	GLN
2	D	35	HIS
2	D	39	GLN
2	D	53	ASN
2	D	54	ASN
2	D	162	ASN

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Mol	Chain	Res	Type
2	D	172	HIS
2	D	209	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 ⓘ

2 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$
3	1PC	B	227	-	19,20,20	3.43	9 (47%)	24,27,27	1.62	3 (12%)
3	1PC	C	212	-	19,20,20	3.36	7 (36%)	24,27,27	1.43	2 (8%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	1PC	B	227	-	-	2/12/30/30	0/3/3/3
3	1PC	C	212	-	-	0/12/30/30	0/3/3/3

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	212	1PC	CH-CG	9.02	1.62	1.54
3	C	212	1PC	CL-CG	7.97	1.61	1.54
3	B	227	1PC	CH-CG	7.15	1.60	1.54
3	B	227	1PC	CN-NM	6.35	1.56	1.47
3	B	227	1PC	CG-CA	6.00	1.60	1.52
3	B	227	1PC	CR-NM	4.92	1.54	1.47
3	C	212	1PC	CN-NM	4.87	1.54	1.47
3	B	227	1PC	CL-CG	4.73	1.58	1.54
3	C	212	1PC	CG-CA	4.00	1.58	1.52
3	B	227	1PC	CF-CA	3.98	1.46	1.39
3	B	227	1PC	CD-CC	3.41	1.45	1.38
3	B	227	1PC	CC-CB	3.20	1.44	1.38
3	C	212	1PC	CR-NM	2.57	1.50	1.47
3	C	212	1PC	CD-CC	2.36	1.43	1.38
3	B	227	1PC	CE-CF	2.27	1.42	1.38
3	C	212	1PC	CJ-CI	2.04	1.59	1.51

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	227	1PC	CL-CG-CH	-5.60	99.57	108.52
3	C	212	1PC	CL-CG-CH	-3.38	103.11	108.52
3	B	227	1PC	CI-CH-CG	-3.32	107.73	113.18
3	C	212	1PC	CI-CH-CG	-3.03	108.21	113.18
3	B	227	1PC	CL-CG-NM	-2.50	104.56	109.86

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	227	1PC	CL-CG-NM-CR
3	B	227	1PC	CL-CG-NM-CN

There are no ring outliers.

2 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	227	1PC	5	0
3	C	212	1PC	8	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	216/216 (100%)	-0.68	1 (0%) 87 85	7, 19, 34, 75	0
1	C	216/216 (100%)	-0.58	0 100 100	4, 22, 35, 57	0
2	B	215/215 (100%)	-0.47	0 100 100	5, 23, 39, 56	0
2	D	215/215 (100%)	-0.48	2 (0%) 81 79	6, 24, 41, 61	0
All	All	862/862 (100%)	-0.55	3 (0%) 90 88	4, 22, 38, 75	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	201	SER	5.7
2	D	129	ALA	2.9
2	D	130	ALA	2.7

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
3	1PC	C	212	18/18	0.90	0.10	3,19,31,31	0
3	1PC	B	227	18/18	0.92	0.06	4,17,26,26	0

6.5 Other polymers [i](#)

There are no such residues in this entry.