



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 02:05 PM UTC

PDB ID : 1KCS / pdb_00001kcs
Title : CRYSTAL STRUCTURE OF ANTIBODY PC282 IN COMPLEX WITH PS1 PEPTIDE
Authors : Nair, D.T.; Singh, K.; Siddiqui, Z.; Nayak, B.P.; Rao, K.V.S.; Salunke, D.M.
Deposited on : 2001-11-11
Resolution : 2.50 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
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

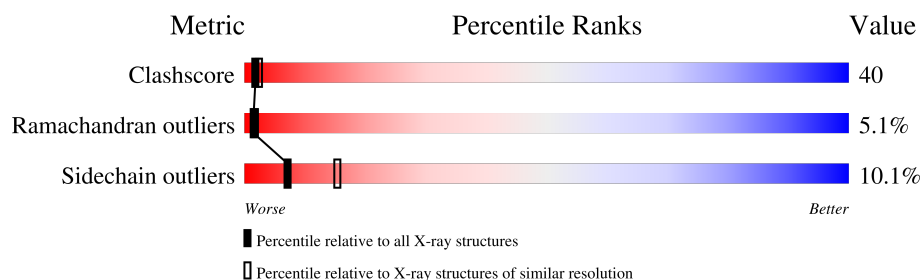
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	L	214	46% 45% 7% .
2	H	217	45% 40% 11% .
3	P	15	40% 7% 53%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 3348 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 PC282 IMMUNOGLOBULIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	214	Total	C	N	O	S	0	0	0
			1611	996	269	337	9			

- Molecule 2 is a protein called PC282 IMMUNOGLOBULIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	217	Total	C	N	O	S	0	0	0
			1600	1010	260	325	5			

- Molecule 3 is a protein called PS1 peptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	P	7	Total	C	N	O	0	0	0
			52	34	8	10			

- Molecule 4 is water.

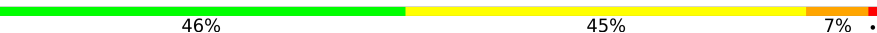
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	L	41	Total	O	0	0
			41	41		
4	H	43	Total	O	0	0
			43	43		
4	P	1	Total	O	0	0
			1	1		

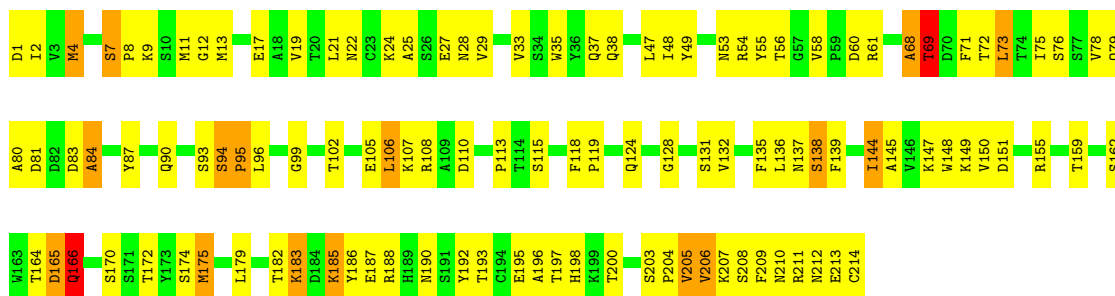
3 Residue-property plots

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. 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. 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.

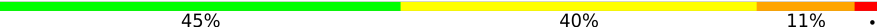
Note EDS was not executed.

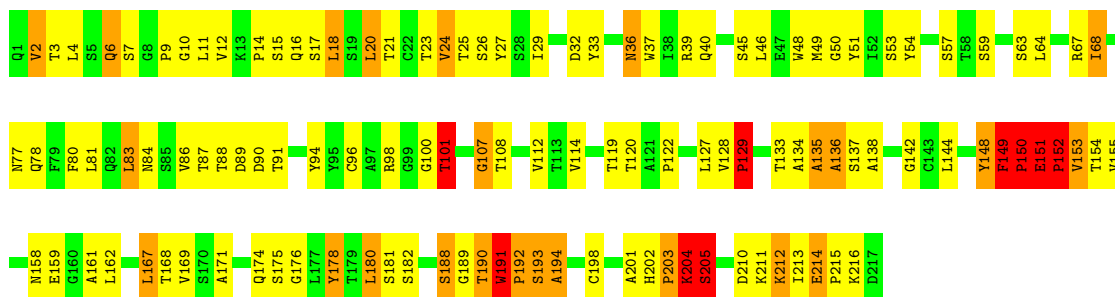
• Molecule 1: PC282 IMMUNOGLOBULIN

Chain L: 



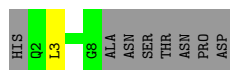
• Molecule 2: PC282 IMMUNOGLOBULIN

Chain H: 



• Molecule 3: PS1 peptide

Chain P: 



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	52.60 Å 69.52 Å 59.36 Å 90.00° 95.62° 90.00°	Depositor
Resolution (Å)	50.00 – 2.50	Depositor
% Data completeness (in resolution range)	84.3 (50.00-2.50)	Depositor
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 0.5	Depositor
R, R_{free}	0.209 , 0.277	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3348	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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	L	0.49	0/1646	1.01	5/2233 (0.2%)
2	H	0.68	1/1640 (0.1%)	2.01	36/2249 (1.6%)
3	P	0.50	0/53	0.73	0/71
All	All	0.59	1/3339 (0.0%)	1.58	41/4553 (0.9%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	191	TRP	N-CA	-5.28	1.38	1.46

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	151	GLU	CA-C-N	45.49	176.71	119.84
2	H	151	GLU	C-N-CA	45.49	176.71	119.84
2	H	149	PHE	CA-C-N	-18.68	96.48	119.84
2	H	149	PHE	C-N-CA	-18.68	96.48	119.84
2	H	152	PRO	CA-N-CD	-15.08	90.89	112.00
2	H	152	PRO	N-CA-CB	10.79	114.58	103.25
2	H	152	PRO	N-CD-CG	10.27	118.61	103.20
2	H	151	GLU	C-N-CD	-9.55	85.85	125.00
2	H	191	TRP	CA-C-N	-8.43	109.71	119.32
2	H	191	TRP	C-N-CA	-8.43	109.71	119.32
2	H	190	THR	CA-C-N	-8.32	101.51	121.80
2	H	190	THR	C-N-CA	-8.32	101.51	121.80
2	H	205	SER	N-CA-C	-8.18	103.32	113.38
2	H	191	TRP	CB-CA-C	7.55	125.04	110.17
2	H	150	PRO	CA-N-CD	-7.46	101.55	112.00
1	L	206	VAL	N-CA-C	7.45	118.84	108.12
2	H	192	PRO	CA-N-CD	-7.19	101.93	112.00
2	H	36	ASN	N-CA-C	7.18	121.55	110.42
2	H	149	PHE	N-CA-C	6.54	124.27	109.81
2	H	189	GLY	CA-C-N	6.18	129.18	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	189	GLY	C-N-CA	6.18	129.18	120.28
2	H	148	TYR	CA-C-N	-6.13	106.84	121.80
2	H	148	TYR	C-N-CA	-6.13	106.84	121.80
2	H	149	PHE	CA-C-O	-6.10	111.80	120.16
2	H	188	SER	CA-C-N	-5.90	113.51	119.94
2	H	188	SER	C-N-CA	-5.90	113.51	119.94
1	L	93	SER	N-CA-C	5.86	119.27	109.95
2	H	101	THR	N-CA-C	-5.70	102.75	110.68
2	H	149	PHE	O-C-N	-5.59	114.89	121.32
2	H	68	ILE	N-CA-C	5.57	117.60	108.97
2	H	107	GLY	N-CA-C	-5.54	103.68	112.66
2	H	136	ALA	CB-CA-C	-5.35	109.95	117.23
1	L	119	PRO	CA-C-N	-5.33	114.47	119.85
1	L	119	PRO	C-N-CA	-5.33	114.47	119.85
1	L	166	GLN	OE1-CD-NE2	-5.29	117.31	122.60
2	H	214	GLU	CA-C-N	5.23	126.38	119.84
2	H	214	GLU	C-N-CA	5.23	126.38	119.84
2	H	189	GLY	O-C-N	5.23	127.21	122.19
2	H	204	LYS	N-CA-C	5.19	118.72	112.38
2	H	178	TYR	N-CA-C	5.16	118.52	110.32
2	H	189	GLY	N-CA-C	-5.09	106.33	112.49

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	L	1611	0	1535	142	0
2	H	1600	0	1555	126	0
3	P	52	0	46	1	0
4	H	43	0	0	13	0
4	L	41	0	0	11	0
4	P	1	0	0	0	0
All	All	3348	0	3136	257	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 40.

All (257) 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:L:94:SER:OG	1:L:95:PRO:HD3	1.29	1.27
1:L:94:SER:OG	1:L:95:PRO:CD	1.86	1.24
1:L:87:TYR:HD1	4:L:222:HOH:O	1.34	1.06
1:L:38:GLN:HE22	2:H:40:GLN:HE22	1.07	1.02
1:L:136:LEU:HD23	1:L:175:MET:HE2	1.39	1.01
1:L:7:SER:HB3	1:L:8:PRO:HD3	1.42	1.00
1:L:37:GLN:HB2	1:L:47:LEU:HD11	1.45	0.96
2:H:3:THR:HG23	2:H:25:THR:HB	1.45	0.95
2:H:122:PRO:HB3	2:H:148:TYR:HB3	1.48	0.95
2:H:91:THR:HG22	2:H:114:VAL:H	1.29	0.95
2:H:39:ARG:HB3	2:H:49:MET:HE2	1.54	0.89
2:H:152:PRO:O	2:H:153:VAL:HG13	1.75	0.86
1:L:137:ASN:HD21	2:H:167:LEU:HD13	1.40	0.84
1:L:144:ILE:HG12	4:L:234:HOH:O	1.78	0.83
2:H:24:VAL:HG13	2:H:77:ASN:ND2	1.94	0.83
2:H:149:PHE:O	2:H:150:PRO:O	1.96	0.82
1:L:1:ASP:CG	1:L:2:ILE:H	1.85	0.82
1:L:94:SER:OG	1:L:95:PRO:HD2	1.77	0.82
1:L:68:ALA:O	1:L:69:THR:HB	1.79	0.81
2:H:88:THR:O	2:H:91:THR:HG23	1.81	0.80
1:L:13:MET:HG3	1:L:19:VAL:HG12	1.63	0.80
2:H:136:ALA:O	2:H:188:SER:HB3	1.84	0.78
1:L:38:GLN:NE2	2:H:40:GLN:HE22	1.81	0.78
1:L:113:PRO:HB3	1:L:139:PHE:HB3	1.63	0.78
1:L:94:SER:HG	1:L:95:PRO:HD3	1.46	0.77
1:L:28:ASN:HD22	1:L:68:ALA:HB1	1.49	0.77
1:L:38:GLN:HE22	2:H:40:GLN:NE2	1.83	0.77
2:H:180:LEU:HD23	2:H:181:SER:N	1.99	0.77
2:H:149:PHE:O	2:H:150:PRO:C	2.12	0.76
1:L:1:ASP:CG	1:L:95:PRO:HG2	2.11	0.75
1:L:137:ASN:ND2	2:H:167:LEU:HD13	2.02	0.75
2:H:98:ARG:HB2	4:H:226:HOH:O	1.87	0.75
2:H:151:GLU:HG3	2:H:178:TYR:CE2	2.22	0.74
1:L:136:LEU:HD23	1:L:175:MET:CE	2.18	0.74
1:L:7:SER:CB	1:L:8:PRO:HD3	2.18	0.74
1:L:190:ASN:HD21	1:L:212:ASN:HB3	1.53	0.73
2:H:149:PHE:C	2:H:150:PRO:O	2.31	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:101:THR:O	2:H:101:THR:CG2	2.35	0.73
2:H:10:GLY:HA3	2:H:204:LYS:HE2	1.71	0.73
2:H:204:LYS:HD2	2:H:204:LYS:N	2.04	0.72
2:H:67:ARG:HH22	2:H:90:ASP:CG	1.97	0.71
2:H:4:LEU:HD11	4:H:226:HOH:O	1.91	0.71
2:H:16:GLN:O	2:H:86:VAL:HG22	1.92	0.69
1:L:113:PRO:HB3	1:L:139:PHE:CD2	2.28	0.69
2:H:91:THR:HG22	2:H:114:VAL:N	2.07	0.68
1:L:145:ALA:HB3	1:L:197:THR:CG2	2.23	0.68
1:L:196:ALA:HB1	4:L:234:HOH:O	1.94	0.67
1:L:12:GLY:HA2	1:L:105:GLU:O	1.93	0.67
1:L:94:SER:CB	1:L:95:PRO:HD3	2.23	0.67
2:H:149:PHE:O	2:H:149:PHE:CD1	2.48	0.67
1:L:164:THR:HG23	1:L:174:SER:O	1.94	0.66
1:L:179:LEU:HD11	4:L:231:HOH:O	1.94	0.66
2:H:108:THR:HG22	2:H:108:THR:O	1.94	0.66
2:H:191:TRP:HZ3	2:H:213:ILE:O	1.78	0.66
2:H:119:THR:HG23	2:H:150:PRO:HD2	1.78	0.66
2:H:202:HIS:ND1	2:H:205:SER:HB3	2.10	0.65
1:L:7:SER:HB3	1:L:8:PRO:CD	2.24	0.65
2:H:100:GLY:HA2	3:P:3:LEU:HD22	1.78	0.65
1:L:145:ALA:HB3	1:L:197:THR:HG22	1.79	0.65
1:L:4:MET:SD	1:L:90:GLN:HB3	2.37	0.64
2:H:36:ASN:OD1	2:H:51:TYR:HB3	1.97	0.64
1:L:8:PRO:HD2	4:L:227:HOH:O	1.97	0.64
1:L:28:ASN:HD22	1:L:68:ALA:CB	2.10	0.64
2:H:17:SER:CB	2:H:84:ASN:HA	2.27	0.64
1:L:1:ASP:HB2	1:L:95:PRO:HG2	1.77	0.64
1:L:1:ASP:CG	1:L:2:ILE:N	2.55	0.64
1:L:48:ILE:HD13	1:L:54:ARG:HA	1.80	0.63
2:H:17:SER:HB3	2:H:84:ASN:HA	1.80	0.63
2:H:4:LEU:HD21	4:H:226:HOH:O	1.97	0.63
1:L:150:VAL:O	1:L:151:ASP:HB2	1.98	0.63
2:H:6:GLN:OE1	2:H:107:GLY:HA3	1.99	0.63
2:H:18:LEU:HD22	2:H:20:LEU:HD21	1.79	0.63
1:L:17:GLU:O	1:L:78:VAL:HG23	1.99	0.63
1:L:165:ASP:OD2	1:L:165:ASP:N	2.32	0.62
2:H:168:THR:HG22	2:H:169:VAL:N	2.14	0.62
1:L:128:GLY:HA2	1:L:183:LYS:HZ2	1.63	0.62
2:H:204:LYS:N	2:H:204:LYS:CD	2.62	0.62
1:L:203:SER:HB2	1:L:204:PRO:HD2	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:1:ASP:CB	1:L:95:PRO:HG2	2.28	0.61
1:L:25:ALA:HB3	1:L:69:THR:HA	1.81	0.61
1:L:175:MET:HE3	1:L:175:MET:C	2.25	0.61
2:H:191:TRP:CZ3	2:H:213:ILE:O	2.54	0.61
2:H:2:VAL:HG21	2:H:98:ARG:NH2	2.16	0.61
2:H:18:LEU:HD23	2:H:112:VAL:HG11	1.82	0.61
2:H:128:VAL:HG22	2:H:213:ILE:CG2	2.30	0.60
1:L:165:ASP:O	1:L:166:GLN:O	2.18	0.60
2:H:14:PRO:O	2:H:15:SER:HB2	2.01	0.60
1:L:137:ASN:HD21	2:H:167:LEU:CD1	2.10	0.60
2:H:6:GLN:NE2	2:H:6:GLN:H	2.00	0.60
1:L:164:THR:HG22	2:H:168:THR:O	2.01	0.60
2:H:149:PHE:O	2:H:149:PHE:CG	2.53	0.59
1:L:8:PRO:O	1:L:102:THR:HG23	2.02	0.59
1:L:19:VAL:HG21	1:L:75:ILE:HD12	1.84	0.59
2:H:101:THR:O	2:H:101:THR:HG22	2.01	0.59
1:L:4:MET:O	1:L:99:GLY:HA2	2.01	0.59
2:H:127:LEU:HB2	2:H:142:GLY:CA	2.32	0.59
2:H:39:ARG:CB	2:H:49:MET:HE2	2.31	0.59
2:H:158:ASN:HB3	2:H:161:ALA:HB3	1.84	0.59
1:L:200:THR:HA	4:L:250:HOH:O	2.02	0.58
2:H:10:GLY:CA	2:H:204:LYS:HE2	2.34	0.58
2:H:24:VAL:HG11	2:H:29:ILE:HG23	1.84	0.58
1:L:128:GLY:HA2	1:L:183:LYS:NZ	2.19	0.58
1:L:110:ASP:HB3	1:L:200:THR:HG22	1.85	0.57
2:H:32:ASP:O	2:H:33:TYR:HB2	2.03	0.57
1:L:79:GLN:HA	1:L:79:GLN:HE21	1.69	0.57
2:H:3:THR:CG2	2:H:25:THR:HB	2.27	0.57
2:H:212:LYS:HE2	2:H:214:GLU:HG2	1.86	0.57
1:L:108:ARG:NH1	1:L:172:THR:HG23	2.19	0.57
1:L:78:VAL:HG12	1:L:106:LEU:HD11	1.85	0.57
1:L:137:ASN:ND2	1:L:138:SER:H	2.04	0.56
1:L:182:THR:OG1	1:L:185:LYS:HG3	2.05	0.56
2:H:20:LEU:N	2:H:20:LEU:HD22	2.21	0.56
2:H:9:PRO:HD2	4:H:228:HOH:O	2.06	0.55
1:L:149:LYS:HB2	1:L:193:THR:HB	1.88	0.55
1:L:19:VAL:HG22	1:L:75:ILE:HB	1.88	0.55
2:H:127:LEU:HB2	2:H:142:GLY:HA3	1.88	0.55
1:L:118:PHE:HE2	2:H:129:PRO:HD3	1.71	0.55
1:L:147:LYS:HD2	1:L:149:LYS:NZ	2.21	0.55
1:L:198:HIS:HD2	1:L:200:THR:OG1	1.90	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:53:SER:OG	2:H:57:SER:HB2	2.07	0.55
2:H:88:THR:HG23	2:H:89:ASP:OD1	2.07	0.55
1:L:49:TYR:O	1:L:53:ASN:HB2	2.07	0.54
2:H:39:ARG:HB3	2:H:49:MET:CE	2.32	0.54
1:L:68:ALA:O	1:L:69:THR:CB	2.55	0.54
1:L:196:ALA:O	1:L:205:VAL:HG23	2.08	0.54
1:L:80:ALA:HA	1:L:106:LEU:HG	1.90	0.54
2:H:48:TRP:CZ2	2:H:50:GLY:HA2	2.43	0.53
1:L:83:ASP:O	1:L:84:ALA:HB2	2.09	0.53
1:L:78:VAL:CG1	1:L:106:LEU:HD11	2.39	0.53
2:H:154:THR:HB	2:H:201:ALA:HB3	1.91	0.53
1:L:72:THR:HG23	4:L:242:HOH:O	2.08	0.52
1:L:162:SER:O	1:L:175:MET:HB2	2.08	0.52
2:H:135:ALA:HB3	2:H:138:ALA:O	2.09	0.52
1:L:12:GLY:O	1:L:13:MET:HE2	2.08	0.52
1:L:54:ARG:HD3	1:L:58:VAL:O	2.09	0.52
1:L:113:PRO:HB3	1:L:139:PHE:HD2	1.73	0.52
1:L:113:PRO:HB3	1:L:139:PHE:CB	2.39	0.52
2:H:129:PRO:O	2:H:216:LYS:HD3	2.10	0.51
1:L:21:LEU:HD12	4:L:225:HOH:O	2.10	0.51
1:L:135:PHE:CE2	1:L:137:ASN:HB2	2.45	0.51
2:H:7:SER:HA	4:H:219:HOH:O	2.10	0.51
1:L:7:SER:CB	1:L:8:PRO:CD	2.88	0.51
1:L:4:MET:HE3	1:L:90:GLN:HG2	1.92	0.51
2:H:49:MET:HE1	2:H:94:TYR:CD2	2.46	0.51
1:L:113:PRO:CB	1:L:139:PHE:HB3	2.36	0.50
2:H:10:GLY:HA3	2:H:204:LYS:CE	2.40	0.50
2:H:37:TRP:CD1	2:H:81:LEU:HB2	2.45	0.50
1:L:108:ARG:HD2	1:L:170:SER:O	2.11	0.50
1:L:209:PHE:C	1:L:210:ASN:HD22	2.19	0.50
2:H:24:VAL:HG11	2:H:29:ILE:CG2	2.40	0.50
2:H:128:VAL:CG2	2:H:213:ILE:HG23	2.42	0.50
2:H:152:PRO:O	2:H:153:VAL:CG1	2.52	0.50
1:L:49:TYR:CD2	2:H:101:THR:HG23	2.46	0.50
2:H:6:GLN:H	2:H:6:GLN:HE21	1.59	0.50
2:H:101:THR:O	2:H:101:THR:HG23	2.10	0.50
2:H:168:THR:HG22	2:H:169:VAL:H	1.75	0.50
2:H:23:THR:HA	2:H:78:GLN:HG2	1.94	0.50
1:L:124:GLN:HE22	1:L:131:SER:H	1.60	0.50
1:L:186:TYR:HA	1:L:192:TYR:OH	2.12	0.49
2:H:40:GLN:HB2	2:H:46:LEU:HD23	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:83:ASP:CG	4:L:241:HOH:O	2.55	0.49
1:L:193:THR:HG23	1:L:208:SER:HB2	1.93	0.49
2:H:169:VAL:O	2:H:180:LEU:HG	2.11	0.49
1:L:1:ASP:HB2	1:L:95:PRO:CG	2.41	0.49
1:L:4:MET:HA	1:L:24:LYS:O	2.12	0.49
1:L:4:MET:HE2	1:L:25:ALA:CB	2.43	0.49
1:L:206:VAL:HG23	1:L:206:VAL:O	2.11	0.49
2:H:128:VAL:HG22	2:H:213:ILE:HG23	1.95	0.49
1:L:61:ARG:HG3	1:L:75:ILE:HG23	1.95	0.48
2:H:51:TYR:CD1	2:H:51:TYR:C	2.91	0.48
1:L:195:GLU:HG3	1:L:206:VAL:HG12	1.94	0.48
2:H:94:TYR:CD1	2:H:94:TYR:N	2.82	0.48
1:L:193:THR:HG23	1:L:207:LYS:O	2.14	0.48
1:L:28:ASN:ND2	1:L:68:ALA:CB	2.76	0.48
2:H:67:ARG:HB3	2:H:83:LEU:CD2	2.43	0.48
2:H:193:SER:OG	2:H:194:ALA:N	2.47	0.48
1:L:61:ARG:O	1:L:75:ILE:HA	2.13	0.48
2:H:216:LYS:HB3	4:H:242:HOH:O	2.14	0.48
1:L:80:ALA:HA	1:L:106:LEU:CD2	2.44	0.48
2:H:168:THR:CG2	2:H:169:VAL:N	2.77	0.48
1:L:211:ARG:HH11	1:L:211:ARG:HG2	1.79	0.48
1:L:54:ARG:NE	1:L:60:ASP:HA	2.28	0.47
1:L:118:PHE:CE2	2:H:129:PRO:HD3	2.49	0.47
1:L:183:LYS:NZ	1:L:183:LYS:HB3	2.30	0.47
2:H:63:SER:OG	2:H:64:LEU:HD12	2.13	0.47
1:L:137:ASN:ND2	1:L:138:SER:N	2.62	0.47
1:L:185:LYS:O	1:L:188:ARG:HG2	2.14	0.47
2:H:26:SER:O	2:H:27:TYR:HB2	2.13	0.47
1:L:49:TYR:CG	2:H:101:THR:HG23	2.49	0.47
2:H:10:GLY:N	2:H:204:LYS:HE2	2.29	0.47
2:H:36:ASN:O	2:H:96:CYS:HA	2.14	0.47
1:L:137:ASN:HD22	1:L:138:SER:H	1.61	0.47
2:H:108:THR:O	2:H:108:THR:CG2	2.62	0.47
2:H:67:ARG:NH2	4:H:229:HOH:O	2.48	0.47
1:L:33:VAL:HG21	1:L:71:PHE:CD1	2.49	0.47
2:H:67:ARG:NH2	2:H:90:ASP:CG	2.70	0.47
2:H:11:LEU:HD13	2:H:12:VAL:N	2.31	0.46
4:L:226:HOH:O	2:H:181:SER:HB3	2.15	0.46
2:H:21:THR:HG23	2:H:80:PHE:CE2	2.51	0.46
2:H:67:ARG:CZ	4:H:229:HOH:O	2.63	0.46
1:L:115:SER:HA	1:L:135:PHE:O	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:79:GLN:HA	1:L:79:GLN:NE2	2.31	0.45
1:L:183:LYS:HG2	1:L:187:GLU:OE2	2.16	0.45
2:H:17:SER:HB2	2:H:84:ASN:HA	1.97	0.45
1:L:4:MET:CE	1:L:25:ALA:HB2	2.47	0.45
1:L:2:ILE:HG12	1:L:27:GLU:HG2	1.99	0.44
1:L:13:MET:HG3	1:L:19:VAL:CG1	2.40	0.44
1:L:35:TRP:CE2	1:L:73:LEU:HB2	2.52	0.44
2:H:14:PRO:O	2:H:15:SER:CB	2.66	0.44
2:H:190:THR:O	2:H:190:THR:CG2	2.62	0.44
1:L:75:ILE:O	1:L:76:SER:C	2.60	0.44
2:H:45:SER:HA	4:H:250:HOH:O	2.16	0.44
2:H:86:VAL:HA	4:H:229:HOH:O	2.17	0.44
2:H:198:CYS:SG	2:H:211:LYS:HB3	2.58	0.44
2:H:6:GLN:HG3	2:H:96:CYS:SG	2.57	0.43
2:H:193:SER:N	4:H:227:HOH:O	2.27	0.43
1:L:94:SER:CB	1:L:95:PRO:CD	2.77	0.43
2:H:171:ALA:HB1	2:H:178:TYR:HD2	1.84	0.43
1:L:55:TYR:CG	1:L:56:THR:N	2.86	0.43
2:H:134:ALA:C	2:H:136:ALA:H	2.26	0.43
1:L:175:MET:HE3	1:L:175:MET:O	2.18	0.42
1:L:132:VAL:HG12	1:L:148:TRP:CH2	2.54	0.42
1:L:190:ASN:ND2	1:L:212:ASN:HB3	2.27	0.42
1:L:207:LYS:O	1:L:208:SER:HB2	2.18	0.42
1:L:19:VAL:HG13	1:L:78:VAL:CG2	2.50	0.42
2:H:18:LEU:HA	4:H:258:HOH:O	2.19	0.42
2:H:24:VAL:HG12	2:H:77:ASN:O	2.19	0.42
1:L:115:SER:HB3	1:L:136:LEU:CD1	2.49	0.42
1:L:144:ILE:O	1:L:144:ILE:CG2	2.66	0.42
1:L:209:PHE:C	1:L:209:PHE:CD1	2.97	0.42
2:H:127:LEU:HD21	2:H:144:LEU:HB2	2.02	0.42
2:H:168:THR:CG2	2:H:169:VAL:H	2.31	0.42
1:L:11:MET:HB2	1:L:11:MET:HE3	1.84	0.42
1:L:48:ILE:HG22	1:L:49:TYR:N	2.35	0.42
2:H:155:VAL:HG11	2:H:182:SER:HB2	2.01	0.42
2:H:190:THR:O	2:H:190:THR:HG22	2.19	0.41
2:H:67:ARG:NH2	2:H:90:ASP:OD2	2.53	0.41
1:L:19:VAL:CG2	1:L:75:ILE:HD12	2.49	0.41
2:H:193:SER:O	2:H:194:ALA:C	2.62	0.41
1:L:22:ASN:HD21	1:L:24:LYS:HE2	1.86	0.41
1:L:87:TYR:CD1	4:L:222:HOH:O	2.25	0.41
1:L:96:LEU:HD12	1:L:96:LEU:H	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:213:GLU:O	1:L:214:CYS:C	2.63	0.41
2:H:153:VAL:HA	2:H:201:ALA:O	2.21	0.41
1:L:13:MET:O	1:L:107:LYS:N	2.52	0.41
1:L:79:GLN:C	1:L:81:ASP:N	2.73	0.41
1:L:115:SER:OG	1:L:207:LYS:HG2	2.20	0.41
1:L:4:MET:HE2	1:L:25:ALA:HB2	2.02	0.41
1:L:4:MET:HE1	1:L:29:VAL:HG11	2.01	0.41
1:L:183:LYS:HB3	1:L:183:LYS:HZ3	1.84	0.41
1:L:79:GLN:O	1:L:106:LEU:HD21	2.20	0.41
1:L:207:LYS:HA	1:L:207:LYS:HD3	1.88	0.41
2:H:32:ASP:HA	2:H:54:TYR:CD2	2.56	0.41
2:H:67:ARG:NE	4:H:229:HOH:O	2.52	0.41
1:L:185:LYS:HE3	1:L:185:LYS:HB3	1.18	0.40
2:H:64:LEU:O	2:H:68:ILE:HG22	2.20	0.40
2:H:174:GLN:O	2:H:175:SER:OG	2.28	0.40

There are no symmetry-related clashes.

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	L	212/214 (99%)	187 (88%)	16 (8%)	9 (4%)	2	2
2	H	215/217 (99%)	186 (86%)	16 (7%)	13 (6%)	1	1
3	P	5/15 (33%)	3 (60%)	2 (40%)	0	100	100
All	All	432/446 (97%)	376 (87%)	34 (8%)	22 (5%)	1	2

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	7	SER
1	L	166	GLN

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Mol	Chain	Res	Type
2	H	152	PRO
2	H	193	SER
2	H	150	PRO
1	L	68	ALA
1	L	69	THR
2	H	137	SER
1	L	94	SER
1	L	138	SER
2	H	133	THR
2	H	194	ALA
2	H	215	PRO
1	L	84	ALA
2	H	135	ALA
2	H	176	GLY
2	H	203	PRO
1	L	95	PRO
2	H	149	PHE
2	H	129	PRO
2	H	153	VAL
1	L	144	ILE

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	L	183/183 (100%)	171 (93%)	12 (7%)	15	32
2	H	179/180 (99%)	154 (86%)	25 (14%)	3	7
3	P	5/12 (42%)	5 (100%)	0	100	100
All	All	367/375 (98%)	330 (90%)	37 (10%)	7	15

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	4	MET
1	L	9	LYS

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Mol	Chain	Res	Type
1	L	69	THR
1	L	73	LEU
1	L	106	LEU
1	L	155	ARG
1	L	159	THR
1	L	165	ASP
1	L	175	MET
1	L	183	LYS
1	L	185	LYS
1	L	205	VAL
2	H	2	VAL
2	H	6	GLN
2	H	18	LEU
2	H	20	LEU
2	H	24	VAL
2	H	59	SER
2	H	83	LEU
2	H	87	THR
2	H	101	THR
2	H	120	THR
2	H	129	PRO
2	H	150	PRO
2	H	151	GLU
2	H	152	PRO
2	H	159	GLU
2	H	162	LEU
2	H	167	LEU
2	H	180	LEU
2	H	191	TRP
2	H	192	PRO
2	H	203	PRO
2	H	204	LYS
2	H	205	SER
2	H	210	ASP
2	H	212	LYS

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

Mol	Chain	Res	Type
1	L	22	ASN
1	L	28	ASN
1	L	38	GLN

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Mol	Chain	Res	Type
1	L	79	GLN
1	L	124	GLN
1	L	137	ASN
1	L	166	GLN
1	L	190	ASN
1	L	198	HIS
1	L	210	ASN
2	H	44	GLN
2	H	82	GLN
2	H	84	ASN
2	H	174	GLN
2	H	183	ASN
3	P	2	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](#)

There are no ligands in this entry.

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

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.