



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 08:55 PM UTC

PDB ID : 1FBI / pdb_00001fbi
Title : CRYSTAL STRUCTURE OF A CROSS-REACTION COMPLEX BETWEEN FAB F9.13.7 AND GUINEA-FOWL LYSOZYME
Authors : Lescar, J.; Alzari, P.M.
Deposited on : 1995-01-19
Resolution : 3.00 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

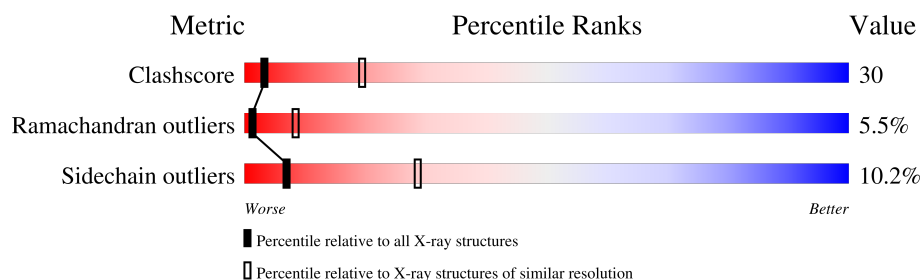
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)

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	49% 45% 7%
1	P	214	46% 46% 7% .
2	H	221	43% 49% 8% .
2	Q	221	51% 42% 7%
3	X	129	44% 44% 10% .
3	Y	129	44% 46% 9% .

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8521 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 IGG1 F9.13.7 FAB (LIGHT CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	214	Total	C	N	O	S	0	0	0
			1641	1023	273	338	7			
1	P	214	Total	C	N	O	S	0	0	0
			1644	1022	271	344	7			

- Molecule 2 is a protein called IGG1 F9.13.7 FAB (HEAVY CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	221	Total	C	N	O	S	0	0	0
			1624	1034	257	326	7			
2	Q	221	Total	C	N	O	S	0	0	0
			1614	1035	253	319	7			

- Molecule 3 is a protein called GUINEA FOWL LYSOZYME.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	X	129	Total	C	N	O	S	0	0	0
			1001	614	193	184	10			
3	Y	129	Total	C	N	O	S	0	0	0
			997	611	192	184	10			

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: IGG1 F9.13.7 FAB (LIGHT CHAIN)



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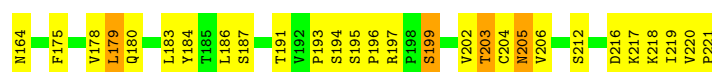
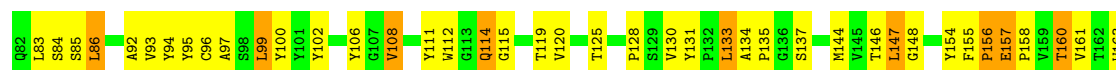


• Molecule 2: IGG1 F9.13.7 FAB (HEAVY CHAIN)

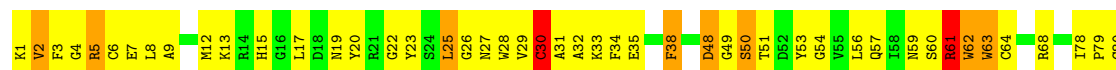




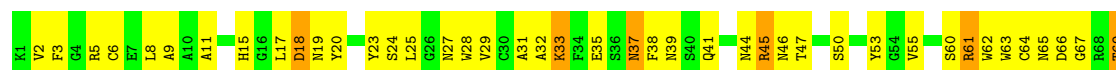
• Molecule 2: IGG1 F9.13.7 FAB (HEAVY CHAIN)



• Molecule 3: GUINEA FOWL LYSOZYME



• Molecule 3: GUINEA FOWL LYSOZYME



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	83.70Å 195.50Å 50.20Å 90.00° 108.50° 90.00°	Depositor
Resolution (Å)	7.00 – 3.00	Depositor
% Data completeness (in resolution range)	(Not available) (7.00-3.00)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.190 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	8521	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.67	0/1676	1.12	12/2277 (0.5%)
1	P	0.55	0/1679	1.01	8/2283 (0.4%)
2	H	0.67	0/1671	1.21	22/2294 (1.0%)
2	Q	0.52	0/1661	0.96	8/2283 (0.4%)
3	X	0.72	0/1022	1.23	7/1379 (0.5%)
3	Y	0.58	0/1018	1.07	6/1375 (0.4%)
All	All	0.62	0/8727	1.10	63/11891 (0.5%)

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	P	0	1

There are no bond length outliers.

All (63) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	X	63	TRP	N-CA-C	11.46	126.77	113.01
2	H	175	PHE	CA-C-N	9.33	129.91	119.83
2	H	175	PHE	C-N-CA	9.33	129.91	119.83
1	L	186	TYR	N-CA-C	-7.64	102.90	111.07
2	H	60	TYR	N-CA-C	7.29	121.30	110.52
1	P	78	LEU	N-CA-C	7.18	121.08	110.30
1	P	7	THR	N-CA-C	6.90	121.31	112.34
3	X	113	LYS	N-CA-C	6.89	118.58	111.14
2	Q	60	TYR	N-CA-C	6.89	119.63	110.53
1	L	58	VAL	CA-C-N	6.83	127.07	119.90
1	L	58	VAL	C-N-CA	6.83	127.07	119.90
1	L	7	THR	N-CA-C	6.80	119.70	111.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	136	LEU	N-CA-C	-6.78	98.97	109.76
2	H	108	VAL	N-CA-C	6.64	116.81	107.37
2	H	126	THR	CA-C-N	6.53	127.10	120.38
2	H	126	THR	C-N-CA	6.53	127.10	120.38
3	X	85	SER	N-CA-C	6.49	118.62	108.96
2	H	96	CYS	N-CA-C	-6.45	99.70	109.95
3	X	56	LEU	N-CA-C	-6.42	100.33	109.96
2	Q	175	PHE	CA-C-N	6.42	126.39	119.78
2	Q	175	PHE	C-N-CA	6.42	126.39	119.78
1	P	5	THR	N-CA-C	6.31	118.99	108.96
3	Y	89	THR	N-CA-C	6.18	118.56	111.02
2	H	195	SER	CA-C-N	6.09	125.71	119.56
2	H	195	SER	C-N-CA	6.09	125.71	119.56
1	L	92	TYR	N-CA-C	6.05	120.21	112.34
1	L	177	SER	N-CA-C	5.92	120.07	112.26
2	H	99	LEU	N-CA-C	-5.90	95.83	107.69
3	Y	69	THR	CA-C-N	5.89	126.08	119.90
3	Y	69	THR	C-N-CA	5.89	126.08	119.90
3	X	30	CYS	N-CA-C	-5.83	104.83	111.07
1	P	82	ASP	N-CA-C	5.80	119.92	112.26
3	Y	37	ASN	N-CA-C	-5.74	104.90	112.24
2	H	30	THR	N-CA-C	5.67	119.30	112.38
2	H	211	SER	N-CA-C	-5.66	105.10	112.23
3	Y	24	SER	N-CA-C	5.64	118.45	110.50
2	H	57	TYR	CA-C-N	5.61	126.09	120.14
2	H	57	TYR	C-N-CA	5.61	126.09	120.14
2	Q	131	TYR	CA-C-N	5.59	126.83	119.84
2	Q	131	TYR	C-N-CA	5.59	126.83	119.84
1	L	93	THR	N-CA-C	5.57	116.70	107.73
2	Q	68	ALA	N-CA-C	5.53	117.43	108.41
1	L	181	LEU	N-CA-C	-5.50	102.03	109.95
2	H	197	ARG	N-CA-C	5.49	114.62	108.25
2	H	102	TYR	N-CA-C	5.49	118.93	110.42
2	H	152	LYS	N-CA-C	5.45	118.46	109.85
2	H	144	MET	N-CA-C	5.43	118.26	109.40
2	H	8	GLY	N-CA-C	5.41	118.77	112.50
1	L	9	SER	N-CA-C	5.33	118.00	111.82
1	P	2	ILE	N-CA-C	-5.31	100.93	108.58
2	H	200	GLU	N-CA-C	5.31	119.01	112.54
3	X	107	ALA	N-CA-C	-5.25	106.13	112.54
2	H	54	SER	N-CA-C	5.21	117.38	111.02
1	L	196	ALA	N-CA-C	5.20	116.80	107.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	Y	53	TYR	N-CA-C	5.20	118.07	109.85
2	H	49	GLY	N-CA-C	5.18	119.05	110.55
2	Q	86	LEU	N-CA-C	5.16	117.37	110.35
1	P	137	ASN	N-CA-C	5.16	118.13	110.14
2	Q	61	ASN	N-CA-C	-5.14	101.59	109.76
3	X	115	CYS	N-CA-C	5.09	121.64	110.80
1	P	170	ASP	N-CA-C	5.08	115.86	108.14
1	P	66	GLY	N-CA-C	5.06	117.19	112.08
1	L	79	GLU	N-CA-C	5.00	114.98	108.07

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	P	50	TYR	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	L	1641	0	1555	106	0
1	P	1644	0	1543	94	0
2	H	1624	0	1541	120	0
2	Q	1614	0	1530	85	0
3	X	1001	0	960	70	0
3	Y	997	0	949	62	0
All	All	8521	0	8078	506	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 30.

All (506) 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:P:159:VAL:HG22	1:P:179:LEU:HD23	1.47	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:49:TYR:HB2	2:H:108:VAL:HG21	1.49	0.94
3:Y:78:ILE:HD12	3:Y:79:PRO:HD2	1.58	0.85
2:Q:14:PRO:HG3	2:Q:120:VAL:HG12	1.59	0.84
2:Q:219:ILE:O	2:Q:221:PRO:HD3	1.81	0.81
3:Y:63:TRP:HB3	3:Y:76:CYS:SG	2.23	0.79
3:Y:31:ALA:HB2	3:Y:111:TRP:HD1	1.48	0.79
2:Q:157:GLU:HG2	2:Q:158:PRO:HA	1.67	0.76
3:X:2:VAL:HA	3:X:38:PHE:O	1.85	0.76
2:Q:39:GLN:O	2:Q:92:ALA:HB1	1.85	0.76
2:H:193:PRO:O	2:H:196:PRO:HD2	1.89	0.73
2:Q:147:LEU:HD12	2:Q:219:ILE:HG21	1.68	0.73
2:Q:195:SER:HB2	2:Q:196:PRO:HD3	1.70	0.73
2:H:39:GLN:O	2:H:92:ALA:HB1	1.89	0.72
3:Y:31:ALA:HB2	3:Y:111:TRP:CD1	2.25	0.72
2:Q:11:LEU:HD23	2:Q:119:THR:HB	1.72	0.72
3:X:34:PHE:CD2	3:X:114:HIS:HD2	2.09	0.71
1:L:130:ALA:HB3	1:L:181:LEU:O	1.90	0.71
1:L:214:CYS:SG	2:H:137:SER:HB3	2.31	0.70
1:L:175:MET:HE2	1:L:177:SER:OG	1.92	0.70
2:H:60:TYR:CE1	2:H:70:LEU:HD23	2.27	0.70
2:H:60:TYR:HE1	2:H:70:LEU:HD23	1.56	0.70
1:P:11:LEU:HB3	1:P:104:LEU:HD23	1.75	0.69
1:P:34:ASN:HB3	1:P:49:TYR:HA	1.74	0.69
2:Q:95:TYR:CD1	2:Q:115:GLY:HA3	2.29	0.68
3:X:93:ASN:HA	3:X:96:LYS:HD2	1.76	0.68
1:L:47:LEU:HA	1:L:58:VAL:HG11	1.75	0.68
1:P:96:TYR:O	2:Q:47:TRP:HB2	1.94	0.68
2:Q:193:PRO:HD2	2:Q:196:PRO:HG2	1.74	0.68
1:P:117:ILE:HD13	1:P:118:PHE:N	2.09	0.67
2:Q:17:SER:HA	2:Q:86:LEU:HD23	1.76	0.67
3:X:34:PHE:CD2	3:X:114:HIS:CD2	2.82	0.67
1:P:29:ILE:HD13	1:P:90:GLN:HB3	1.77	0.67
1:L:89:GLN:HG2	1:L:90:GLN:N	2.11	0.66
1:P:167:ASP:HB3	1:P:170:ASP:O	1.96	0.66
1:L:151:ASP:HB2	1:L:189:HIS:HB3	1.77	0.66
1:P:142:LYS:HZ1	1:P:163:TRP:CD1	2.14	0.66
1:L:89:GLN:HB2	1:L:98:PHE:CD2	2.32	0.65
3:Y:5:ARG:HG2	3:Y:38:PHE:CE2	2.31	0.65
3:Y:25:LEU:O	3:Y:29:VAL:HG23	1.96	0.65
3:Y:19:ASN:HA	3:Y:23:TYR:O	1.95	0.65
2:Q:157:GLU:CG	2:Q:158:PRO:HA	2.27	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:128:PRO:HB3	2:H:154:TYR:HB3	1.78	0.64
3:X:119:ASP:OD1	3:X:121:ARG:HD3	1.96	0.64
2:Q:2:VAL:HB	2:Q:111:TYR:CE1	2.32	0.64
3:X:34:PHE:HD2	3:X:114:HIS:HD2	1.43	0.64
2:Q:81:MET:HE3	2:Q:83:LEU:HD21	1.80	0.64
2:Q:30:THR:HA	2:Q:53:PRO:HB2	1.79	0.64
1:P:133:VAL:HG21	2:Q:133:LEU:HD21	1.79	0.64
2:H:30:THR:HA	2:H:53:PRO:HB2	1.79	0.64
3:Y:61:ARG:O	3:Y:61:ARG:HD3	1.97	0.63
1:P:10:SER:HA	1:P:103:LYS:O	1.99	0.63
3:X:59:ASN:OD1	3:X:60:SER:N	2.31	0.63
1:L:142:LYS:HE3	1:L:163:TRP:CD1	2.34	0.63
2:Q:2:VAL:HG13	2:Q:27:TYR:HD2	1.64	0.63
2:Q:29:PHE:CD2	2:Q:77:SER:HA	2.34	0.63
1:L:39:LYS:HE2	1:L:81:GLU:HB2	1.80	0.62
3:X:23:TYR:CD2	3:X:105:MET:SD	2.93	0.62
1:P:142:LYS:HZ1	1:P:163:TRP:HD1	1.45	0.62
2:Q:15:GLY:O	2:Q:85:SER:HA	1.99	0.62
3:Y:27:ASN:HD22	3:Y:111:TRP:HZ2	1.47	0.62
1:L:160:LEU:HD21	2:H:178:VAL:HG11	1.82	0.62
2:Q:155:PHE:HB2	2:Q:183:LEU:HD23	1.82	0.61
2:Q:163:TRP:CZ3	2:Q:204:CYS:HB3	2.35	0.61
3:Y:20:TYR:CE2	3:Y:96:LYS:HD3	2.36	0.61
3:X:17:LEU:HD22	3:X:28:TRP:CE2	2.36	0.61
1:P:4:MET:HE2	1:P:90:GLN:N	2.15	0.61
2:H:48:ILE:CD1	2:H:81:MET:SD	2.89	0.61
1:L:38:LYS:O	1:L:84:ALA:HB1	2.01	0.61
3:X:51:THR:HB	3:X:53:TYR:CE1	2.35	0.61
2:Q:186:LEU:HD23	2:Q:187:SER:N	2.16	0.61
2:H:149:CYS:SG	2:H:163:TRP:CH2	2.94	0.60
3:Y:11:ALA:HB1	3:Y:88:ILE:HG21	1.82	0.60
1:P:61:ARG:HD2	1:P:76:ARG:O	2.02	0.60
2:H:12:VAL:HG11	2:H:86:LEU:HD12	1.84	0.60
2:H:78:THR:HG23	2:H:80:TYR:HE1	1.66	0.60
2:H:139:ALA:O	2:H:141:THR:N	2.34	0.60
2:Q:30:THR:HG23	2:Q:54:SER:HB3	1.84	0.60
1:L:4:MET:SD	1:L:25:ALA:HB2	2.42	0.59
3:Y:60:SER:HA	3:Y:64:CYS:HB3	1.83	0.59
3:X:38:PHE:N	3:X:38:PHE:CD1	2.69	0.59
1:P:11:LEU:HB3	1:P:104:LEU:CD2	2.33	0.59
1:L:160:LEU:HD21	2:H:178:VAL:CG1	2.32	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:147:LEU:HG	2:H:219:ILE:HG21	1.85	0.59
2:Q:35:HIS:CE1	2:Q:50:GLU:HG3	2.36	0.59
1:P:7:THR:HG23	1:P:8:THR:HG23	1.84	0.59
1:P:181:LEU:HD23	1:P:182:THR:H	1.68	0.59
3:Y:5:ARG:HA	3:Y:38:PHE:HE2	1.68	0.59
1:L:21:ILE:HD12	1:L:21:ILE:N	2.18	0.58
2:H:147:LEU:HB3	2:H:219:ILE:HG21	1.84	0.58
1:L:155:ARG:HG2	1:L:155:ARG:HH11	1.69	0.58
3:Y:2:VAL:HA	3:Y:39:ASN:HA	1.85	0.58
2:H:197:ARG:NH2	2:H:221:PRO:HD3	2.19	0.58
1:L:38:LYS:HG3	1:L:44:VAL:HG22	1.85	0.58
1:L:186:TYR:CD1	1:L:192:TYR:HE2	2.21	0.58
2:H:132:PRO:HD3	2:H:217:LYS:HG2	1.84	0.58
2:H:163:TRP:HB3	2:H:168:LEU:HD23	1.85	0.58
2:Q:161:VAL:HG22	2:Q:206:VAL:HG12	1.84	0.58
3:Y:78:ILE:CD1	3:Y:79:PRO:HD2	2.33	0.58
1:P:19:VAL:CG2	1:P:75:ILE:HB	2.33	0.58
2:H:193:PRO:C	2:H:196:PRO:HD2	2.28	0.57
1:P:193:THR:CG2	1:P:206:VAL:HB	2.34	0.57
1:L:117:ILE:HG22	1:L:207:LYS:HG3	1.85	0.57
2:H:48:ILE:HD13	2:H:81:MET:SD	2.45	0.57
2:H:160:THR:HB	2:H:207:ALA:HB3	1.86	0.57
2:H:29:PHE:CD2	2:H:77:SER:HA	2.39	0.57
1:P:131:SER:OG	1:P:180:THR:HG23	2.04	0.57
1:L:92:TYR:O	1:L:93:THR:HB	2.03	0.57
1:P:89:GLN:HB3	1:P:98:PHE:CD2	2.39	0.57
3:Y:73:ARG:HB3	3:Y:75:LEU:HD21	1.86	0.57
1:P:150:ILE:HD12	1:P:151:ASP:N	2.19	0.57
1:P:151:ASP:HB2	1:P:189:HIS:HB3	1.87	0.57
3:X:60:SER:HA	3:X:64:CYS:HB3	1.86	0.57
3:Y:93:ASN:HA	3:Y:96:LYS:HE3	1.86	0.57
1:P:49:TYR:HB2	2:Q:108:VAL:HG21	1.86	0.57
1:P:39:LYS:HD2	1:P:84:ALA:HB2	1.85	0.56
3:Y:73:ARG:HH21	3:Y:75:LEU:HD11	1.70	0.56
3:Y:113:LYS:O	3:Y:114:HIS:HB3	2.05	0.56
2:H:153:GLY:O	2:H:183:LEU:HD22	2.05	0.56
2:H:151:VAL:HG13	2:H:186:LEU:HB3	1.85	0.56
3:X:12:MET:O	3:X:17:LEU:HB2	2.04	0.56
1:L:29:ILE:HD12	1:L:90:GLN:HB2	1.88	0.56
2:Q:60:TYR:CE1	2:Q:70:LEU:HD23	2.41	0.56
2:H:128:PRO:HD3	2:H:208:HIS:CD2	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:X:33:LYS:HG2	3:X:123:TRP:CH2	2.41	0.56
3:Y:113:LYS:NZ	3:Y:114:HIS:HB2	2.20	0.56
2:H:220:VAL:HG22	2:H:221:PRO:HD2	1.88	0.56
3:X:61:ARG:HG3	3:X:61:ARG:HH11	1.70	0.56
3:X:119:ASP:O	3:X:122:VAL:HG22	2.06	0.56
1:P:164:THR:HB	1:P:174:SER:H	1.69	0.56
1:P:125:LEU:HD23	1:P:129:GLY:O	2.06	0.55
1:P:12:SER:HB3	1:P:105:GLU:OE2	2.06	0.55
3:X:5:ARG:HH11	3:X:123:TRP:C	2.14	0.55
3:Y:73:ARG:HB3	3:Y:75:LEU:CD2	2.36	0.55
2:H:2:VAL:H	2:H:26:GLY:HA3	1.71	0.55
1:P:49:TYR:CE2	2:Q:102:TYR:HE2	2.25	0.55
2:H:197:ARG:HB2	2:H:197:ARG:NH1	2.21	0.55
3:X:51:THR:HB	3:X:53:TYR:HE1	1.72	0.55
3:Y:113:LYS:HZ3	3:Y:114:HIS:HB2	1.70	0.55
2:Q:2:VAL:HG13	2:Q:27:TYR:CD2	2.42	0.55
2:Q:205:ASN:HA	2:Q:216:ASP:HA	1.88	0.54
3:X:1:LYS:HE2	3:X:3:PHE:CE2	2.42	0.54
1:P:33:LEU:HD12	1:P:89:GLN:O	2.08	0.54
2:H:19:LYS:HG3	2:H:82:GLN:HG3	1.89	0.54
3:Y:46:ASN:HB3	3:Y:50:SER:O	2.06	0.54
1:L:166:GLN:HG3	1:L:171:SER:HA	1.89	0.54
3:X:20:TYR:OH	3:X:96:LYS:HB3	2.07	0.54
3:X:34:PHE:HD2	3:X:114:HIS:CD2	2.23	0.54
1:P:50:TYR:O	1:P:51:THR:HB	2.08	0.54
3:Y:3:PHE:HB3	3:Y:8:LEU:HB2	1.90	0.54
1:L:19:VAL:HG11	1:L:104:LEU:HD21	1.89	0.54
2:H:157:GLU:HB3	2:H:158:PRO:HA	1.90	0.54
3:Y:95:ALA:HA	3:Y:98:ILE:HD12	1.90	0.54
3:X:48:ASP:O	3:X:50:SER:N	2.40	0.54
2:Q:39:GLN:HB3	2:Q:93:VAL:HB	1.89	0.54
2:H:123:ALA:HB2	2:H:182:ASP:CB	2.37	0.54
1:P:58:VAL:HG13	1:P:62:PHE:HD2	1.72	0.54
3:X:3:PHE:HA	3:X:7:GLU:OE1	2.08	0.53
1:L:49:TYR:HB2	2:H:108:VAL:CG2	2.33	0.53
3:Y:84:GLN:O	3:Y:84:GLN:HG3	2.08	0.53
1:L:135:PHE:HB3	1:L:137:ASN:ND2	2.24	0.53
1:L:187:GLU:HG2	1:L:211:ARG:NH2	2.23	0.53
1:P:4:MET:SD	1:P:25:ALA:HB2	2.48	0.53
2:H:10:GLU:HG2	2:H:18:VAL:HG21	1.91	0.53
1:P:118:PHE:HB2	1:P:133:VAL:HB	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:62:GLU:O	2:Q:65:LYS:HG3	2.09	0.53
3:X:1:LYS:HG2	3:X:2:VAL:N	2.24	0.53
1:P:16:GLY:C	1:P:77:ASN:HA	2.34	0.53
2:Q:97:ALA:HB2	2:Q:112:TRP:HA	1.89	0.53
3:X:105:MET:C	3:X:107:ALA:H	2.16	0.53
2:Q:16:ALA:O	2:Q:86:LEU:HD23	2.09	0.53
3:Y:113:LYS:HA	3:Y:116:LYS:HD2	1.91	0.53
1:P:115:VAL:HG12	1:P:116:SER:N	2.24	0.52
3:Y:15:HIS:HD2	3:Y:88:ILE:HG23	1.74	0.52
2:Q:60:TYR:HE1	2:Q:70:LEU:HB2	1.74	0.52
3:Y:15:HIS:CD2	3:Y:88:ILE:HG23	2.44	0.52
1:L:35:TRP:CZ3	1:L:88:CYS:HB3	2.44	0.52
2:H:197:ARG:HA	2:H:199:SER:N	2.24	0.52
1:L:65:SER:OG	1:L:66:GLY:N	2.42	0.52
2:H:48:ILE:HD11	2:H:68:ALA:CB	2.40	0.52
2:Q:4:LEU:HD22	2:Q:22:CYS:SG	2.50	0.52
3:X:4:GLY:O	3:X:7:GLU:N	2.42	0.52
3:X:5:ARG:HA	3:X:38:PHE:CE2	2.45	0.52
1:P:4:MET:O	1:P:99:GLY:HA2	2.09	0.52
1:L:175:MET:N	2:H:175:PHE:HE2	2.08	0.52
1:L:163:TRP:O	2:H:176:PRO:HG2	2.10	0.52
2:H:186:LEU:HG	2:H:187:SER:H	1.75	0.52
1:P:110:ASP:HA	1:P:140:TYR:O	2.10	0.52
2:H:203:THR:HG22	2:H:217:LYS:O	2.09	0.52
1:L:10:SER:HA	1:L:103:LYS:O	2.10	0.51
1:L:150:ILE:O	1:L:150:ILE:HG13	2.10	0.51
3:X:26:GLY:HA3	3:X:120:VAL:HG23	1.92	0.51
1:P:165:ASP:O	1:P:173:TYR:CD1	2.63	0.51
2:H:35:HIS:CE1	2:H:50:GLU:HG3	2.45	0.51
3:X:35:GLU:HG3	3:X:57:GLN:HG2	1.92	0.51
2:Q:17:SER:HA	2:Q:86:LEU:CD2	2.40	0.51
1:L:34:ASN:ND2	2:H:108:VAL:HG22	2.25	0.51
3:Y:63:TRP:O	3:Y:76:CYS:HB2	2.11	0.51
1:L:142:LYS:O	1:L:142:LYS:HG2	2.11	0.51
1:P:125:LEU:HD22	1:P:183:LYS:HG3	1.93	0.51
1:P:164:THR:O	1:P:173:TYR:HD1	1.94	0.51
1:P:179:LEU:HD13	1:P:179:LEU:O	2.11	0.51
1:L:186:TYR:CD1	1:L:192:TYR:CE2	2.99	0.51
2:Q:155:PHE:HA	2:Q:156:PRO:O	2.11	0.51
3:X:20:TYR:CZ	3:X:96:LYS:HB3	2.47	0.50
1:P:118:PHE:CD2	2:Q:133:LEU:HB3	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:133:VAL:HG12	1:P:134:CYS:H	1.75	0.50
1:P:115:VAL:HB	1:P:207:LYS:HD3	1.93	0.50
1:P:142:LYS:NZ	1:P:163:TRP:HB3	2.25	0.50
1:P:82:ASP:HB2	1:P:86:TYR:OH	2.11	0.50
2:H:172:VAL:HG12	2:H:173:HIS:N	2.27	0.50
3:Y:20:TYR:CE1	3:Y:96:LYS:HB3	2.47	0.50
3:X:13:LYS:HD3	3:X:129:LEU:HB3	1.92	0.50
3:X:28:TRP:CE3	3:X:105:MET:HE3	2.46	0.50
1:P:155:ARG:NE	1:P:157:ASN:HB3	2.26	0.50
2:Q:38:LYS:HE3	2:Q:94:TYR:CE1	2.46	0.50
3:Y:5:ARG:HA	3:Y:38:PHE:CE2	2.45	0.50
2:H:152:LYS:HB2	2:H:185:THR:HG23	1.93	0.49
1:P:98:PHE:N	1:P:98:PHE:CD1	2.79	0.49
3:Y:109:VAL:HG22	3:Y:110:ALA:N	2.27	0.49
3:Y:113:LYS:HA	3:Y:116:LYS:NZ	2.27	0.49
2:H:154:TYR:HD1	2:H:154:TYR:H	1.60	0.49
3:X:4:GLY:O	3:X:5:ARG:C	2.54	0.49
3:Y:32:ALA:HB1	3:Y:55:VAL:HG22	1.95	0.49
1:L:198:HIS:ND1	1:L:200:THR:OG1	2.45	0.49
2:H:50:GLU:HB3	2:H:59:ASN:HB3	1.93	0.49
1:P:135:PHE:HB3	1:P:137:ASN:ND2	2.28	0.49
1:P:206:VAL:C	1:P:207:LYS:HD2	2.36	0.49
2:H:50:GLU:O	2:H:58:PRO:HA	2.13	0.49
3:X:15:HIS:HD2	3:X:89:THR:HA	1.75	0.49
3:X:94:CYS:O	3:X:94:CYS:SG	2.71	0.49
2:Q:38:LYS:HG3	2:Q:94:TYR:CE1	2.47	0.49
2:Q:144:MET:HE3	2:Q:191:THR:HG22	1.94	0.49
2:Q:163:TRP:HZ3	2:Q:219:ILE:HG13	1.77	0.49
1:L:37:GLN:HB2	1:L:47:LEU:HD11	1.95	0.49
2:Q:17:SER:OG	2:Q:84:SER:HA	2.13	0.49
1:L:116:SER:O	1:L:118:PHE:CE1	2.66	0.49
1:L:135:PHE:CE2	2:H:189:SER:HB3	2.48	0.49
2:H:138:ALA:O	2:H:139:ALA:HB3	2.13	0.49
2:Q:99:LEU:HG	2:Q:108:VAL:O	2.12	0.49
2:H:135:PRO:HG3	2:H:145:VAL:CG1	2.43	0.48
1:P:39:LYS:CD	1:P:84:ALA:HB2	2.42	0.48
1:L:115:VAL:HG22	1:L:136:LEU:HD13	1.94	0.48
2:H:19:LYS:N	2:H:19:LYS:HD2	2.28	0.48
2:H:55:ASP:HB2	3:X:96:LYS:NZ	2.28	0.48
2:H:130:VAL:O	2:H:131:TYR:HD1	1.96	0.48
1:L:133:VAL:CG2	2:H:150:LEU:HD13	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:154:TYR:CE2	2:H:159:VAL:HB	2.48	0.48
3:X:48:ASP:C	3:X:50:SER:H	2.21	0.48
2:Q:95:TYR:CE1	2:Q:115:GLY:HA3	2.48	0.48
3:X:26:GLY:HA3	3:X:120:VAL:CG2	2.44	0.48
3:X:35:GLU:HG3	3:X:57:GLN:CG	2.44	0.48
1:P:133:VAL:HG12	1:P:134:CYS:N	2.29	0.48
3:Y:113:LYS:HA	3:Y:116:LYS:CE	2.43	0.48
1:L:111:ALA:O	1:L:200:THR:HG21	2.13	0.48
1:P:135:PHE:HB3	1:P:137:ASN:HD21	1.78	0.48
2:Q:35:HIS:CD2	2:Q:47:TRP:HE1	2.32	0.48
1:L:54:LEU:HD13	1:L:58:VAL:HG23	1.95	0.48
2:H:197:ARG:HB2	2:H:197:ARG:HH11	1.79	0.48
3:X:9:ALA:HB2	3:X:29:VAL:HG21	1.95	0.48
2:Q:38:LYS:HB2	2:Q:48:ILE:HD11	1.94	0.48
2:Q:160:THR:O	2:Q:206:VAL:HA	2.14	0.48
1:L:150:ILE:HG21	1:L:181:LEU:HD21	1.96	0.47
2:H:209:PRO:O	2:H:210:ALA:HB2	2.14	0.47
2:Q:33:TRP:CZ3	2:Q:52:ASP:HB2	2.49	0.47
2:Q:55:ASP:HB2	3:Y:96:LYS:HZ3	1.79	0.47
1:L:55:HIS:ND1	1:L:56:SER:N	2.62	0.47
2:H:71:THR:CG2	2:H:72:VAL:N	2.77	0.47
1:P:3:GLN:O	1:P:25:ALA:HA	2.14	0.47
1:P:148:TRP:O	1:P:154:GLU:HA	2.14	0.47
3:Y:17:LEU:O	3:Y:18:ASP:C	2.57	0.47
3:Y:96:LYS:O	3:Y:99:VAL:HG12	2.15	0.47
1:L:198:HIS:O	1:L:200:THR:N	2.47	0.47
1:L:186:TYR:CE1	1:L:192:TYR:CE2	3.03	0.47
1:L:49:TYR:CZ	1:L:53:ARG:HD2	2.49	0.47
1:L:193:THR:CG2	1:L:208:SER:HB3	2.44	0.47
1:P:50:TYR:CD1	2:Q:106:TYR:CE1	3.03	0.47
2:H:164:ASN:HB2	2:H:168:LEU:HB3	1.94	0.47
2:Q:205:ASN:OD1	2:Q:205:ASN:N	2.48	0.47
3:Y:31:ALA:O	3:Y:35:GLU:HG2	2.15	0.47
1:P:187:GLU:O	1:P:211:ARG:NH1	2.48	0.47
2:Q:54:SER:OG	3:Y:20:TYR:HE2	1.96	0.47
1:L:89:GLN:HG2	1:L:90:GLN:H	1.79	0.47
2:H:175:PHE:N	2:H:175:PHE:CD1	2.82	0.47
1:L:133:VAL:HG12	1:L:134:CYS:N	2.29	0.47
1:L:29:ILE:HD11	1:L:33:LEU:HD23	1.96	0.47
2:H:133:LEU:HB2	2:H:148:GLY:C	2.41	0.46
1:L:124:GLN:HB2	2:H:131:TYR:CE2	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:179:LEU:HB2	2:H:184:TYR:CD1	2.51	0.46
3:X:19:ASN:O	3:X:22:GLY:N	2.41	0.46
1:P:148:TRP:CH2	1:P:194:CYS:HB2	2.50	0.46
3:Y:5:ARG:O	3:Y:6:CYS:HB2	2.15	0.46
3:X:31:ALA:O	3:X:35:GLU:HB2	2.15	0.46
2:Q:163:TRP:CH2	2:Q:204:CYS:HB3	2.50	0.46
1:L:132:VAL:HG13	1:L:209:PHE:HE2	1.81	0.46
1:P:49:TYR:CZ	1:P:53:ARG:HD2	2.51	0.46
2:Q:178:VAL:HG12	2:Q:179:LEU:N	2.31	0.46
3:X:34:PHE:HE1	3:X:123:TRP:CZ2	2.33	0.46
2:Q:27:TYR:HB2	2:Q:100:TYR:HE2	1.80	0.46
2:Q:148:GLY:HA2	2:Q:163:TRP:CH2	2.49	0.46
2:H:12:VAL:HG12	2:H:13:LYS:O	2.16	0.46
2:H:130:VAL:O	2:H:131:TYR:CD1	2.68	0.46
2:Q:220:VAL:HG13	2:Q:220:VAL:O	2.15	0.46
1:L:58:VAL:HA	1:L:59:PRO:HD3	1.75	0.46
2:H:195:SER:CB	2:H:196:PRO:HD3	2.46	0.46
1:P:206:VAL:O	1:P:207:LYS:HD2	2.16	0.46
3:X:78:ILE:HG13	3:X:79:PRO:HD2	1.98	0.46
2:Q:35:HIS:HD2	2:Q:47:TRP:HE1	1.64	0.46
2:H:72:VAL:HG12	2:H:73:ASP:N	2.31	0.45
1:P:38:LYS:NZ	2:Q:39:GLN:HG2	2.31	0.45
3:Y:83:LEU:HD22	3:Y:91:THR:HA	1.98	0.45
1:L:115:VAL:O	1:L:116:SER:HB3	2.16	0.45
3:X:19:ASN:N	3:X:23:TYR:O	2.49	0.45
1:P:28:ASP:HA	1:P:68:GLY:O	2.16	0.45
2:Q:34:MET:HB3	2:Q:51:ILE:CG2	2.45	0.45
3:Y:60:SER:OG	3:Y:80:CYS:SG	2.61	0.45
1:L:115:VAL:HG21	1:L:205:ILE:CG2	2.47	0.45
1:L:131:SER:HA	1:L:179:LEU:O	2.16	0.45
1:L:190:ASN:OD1	1:L:211:ARG:HG3	2.16	0.45
2:H:145:VAL:HG23	2:H:194:SER:HA	1.99	0.45
2:H:175:PHE:O	2:H:186:LEU:HD12	2.16	0.45
3:X:15:HIS:CD2	3:X:89:THR:HA	2.51	0.45
1:L:193:THR:HG22	1:L:208:SER:HB3	1.99	0.45
2:H:27:TYR:CB	2:H:100:TYR:HE2	2.29	0.45
3:X:38:PHE:N	3:X:38:PHE:HD1	2.13	0.45
1:P:29:ILE:HD13	1:P:90:GLN:CB	2.44	0.45
1:L:187:GLU:HA	1:L:211:ARG:NH1	2.31	0.45
2:H:208:HIS:CD2	2:H:211:SER:OG	2.70	0.45
1:P:15:LEU:HA	1:P:78:LEU:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:107:LYS:HA	1:P:140:TYR:OH	2.17	0.45
1:L:136:LEU:N	1:L:136:LEU:CD2	2.79	0.45
2:H:12:VAL:O	2:H:120:VAL:HA	2.16	0.45
3:X:1:LYS:HG2	3:X:2:VAL:H	1.81	0.45
3:X:54:GLY:O	3:X:57:GLN:NE2	2.50	0.45
3:X:105:MET:C	3:X:107:ALA:N	2.73	0.45
1:P:146:VAL:HG21	1:P:161:ASN:HD21	1.82	0.45
2:Q:39:GLN:HB3	2:Q:93:VAL:O	2.17	0.45
1:L:155:ARG:HG2	1:L:155:ARG:NH1	2.32	0.44
2:H:159:VAL:HA	2:H:207:ALA:O	2.16	0.44
2:Q:4:LEU:HD21	2:Q:34:MET:HE1	1.99	0.44
1:L:130:ALA:O	1:L:180:THR:HA	2.17	0.44
2:H:71:THR:HG22	2:H:72:VAL:N	2.31	0.44
1:P:19:VAL:HG22	1:P:75:ILE:HB	1.99	0.44
1:P:91:GLY:HA2	1:P:96:TYR:CD1	2.53	0.44
2:Q:179:LEU:HD23	2:Q:184:TYR:HE1	1.81	0.44
2:H:18:VAL:C	2:H:19:LYS:HD2	2.43	0.44
1:P:117:ILE:HD12	1:P:209:PHE:HB2	1.99	0.44
3:Y:19:ASN:OD1	3:Y:23:TYR:N	2.51	0.44
3:Y:88:ILE:HG13	3:Y:92:ALA:HB2	1.98	0.44
1:L:159:VAL:HG12	1:L:160:LEU:N	2.32	0.44
1:P:11:LEU:HD23	1:P:104:LEU:HD21	1.98	0.44
1:P:119:PRO:HG3	1:P:209:PHE:CD1	2.53	0.44
2:Q:128:PRO:HB3	2:Q:154:TYR:HB3	2.00	0.44
2:Q:203:THR:HG22	2:Q:218:LYS:HA	1.98	0.44
2:H:37:VAL:CG2	2:H:112:TRP:HZ3	2.31	0.44
2:H:91:SER:OG	2:H:120:VAL:HG13	2.17	0.44
2:Q:47:TRP:CZ2	2:Q:50:GLU:HB2	2.52	0.44
1:L:33:LEU:HG	1:L:71:TYR:CG	2.52	0.44
2:H:204:CYS:O	2:H:216:ASP:HA	2.18	0.44
3:X:1:LYS:HD2	3:X:86:SER:HA	1.99	0.44
2:Q:38:LYS:HE3	2:Q:94:TYR:OH	2.17	0.44
3:Y:11:ALA:HB1	3:Y:88:ILE:CG2	2.48	0.44
1:L:46:LEU:HD22	2:H:110:ASP:HB3	2.00	0.44
2:H:159:VAL:HG12	2:H:186:LEU:HD22	1.98	0.44
3:X:85:SER:OG	3:X:86:SER:N	2.51	0.44
1:L:155:ARG:HH12	1:L:181:LEU:HG	1.83	0.43
1:L:212:ASN:O	1:L:212:ASN:ND2	2.50	0.43
2:H:147:LEU:HD11	2:H:197:ARG:CD	2.48	0.43
3:Y:17:LEU:O	3:Y:28:TRP:NE1	2.51	0.43
1:L:124:GLN:HG3	2:H:131:TYR:CE2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:186:TYR:CE1	1:L:192:TYR:HE2	2.35	0.43
2:H:36:TRP:O	2:H:48:ILE:HG23	2.18	0.43
1:P:117:ILE:HD13	1:P:117:ILE:C	2.43	0.43
3:Y:37:ASN:O	3:Y:38:PHE:HB2	2.19	0.43
3:Y:60:SER:O	3:Y:69:THR:HG21	2.19	0.43
1:L:130:ALA:HB3	1:L:181:LEU:C	2.44	0.43
2:H:168:LEU:O	2:H:170:SER:N	2.51	0.43
1:P:96:TYR:HB2	2:Q:47:TRP:CD1	2.53	0.43
1:P:142:LYS:HZ1	1:P:163:TRP:HB3	1.82	0.43
1:P:142:LYS:O	1:P:144:ILE:HG22	2.18	0.43
2:Q:134:ALA:HB1	2:Q:221:PRO:HA	2.01	0.43
3:Y:64:CYS:SG	3:Y:83:LEU:HD12	2.58	0.43
3:X:54:GLY:HA2	3:X:83:LEU:O	2.18	0.43
1:L:169:LYS:HA	1:L:169:LYS:HD3	1.86	0.43
1:L:203:SER:HA	1:L:204:PRO:HD2	1.84	0.43
2:H:175:PHE:HA	2:H:176:PRO:HD3	1.70	0.43
2:H:197:ARG:HB2	2:H:198:PRO:HA	2.00	0.43
1:L:145:ASN:HB3	1:L:197:THR:OG1	2.18	0.43
2:Q:194:SER:O	2:Q:197:ARG:O	2.37	0.43
1:L:175:MET:HE3	1:L:175:MET:HB2	1.79	0.43
2:H:37:VAL:HG21	2:H:112:TRP:CH2	2.54	0.43
2:H:69:THR:O	2:H:69:THR:HG22	2.18	0.43
2:H:37:VAL:HG22	2:H:95:TYR:HB2	2.00	0.43
2:H:215:VAL:HG12	2:H:216:ASP:N	2.32	0.43
2:Q:178:VAL:O	2:Q:184:TYR:HA	2.18	0.43
1:L:182:THR:O	1:L:183:LYS:C	2.62	0.43
3:Y:66:ASP:HB3	3:Y:80:CYS:SG	2.59	0.43
3:X:27:ASN:HB3	3:X:111:TRP:HE1	1.84	0.42
1:L:39:LYS:CE	1:L:81:GLU:HB2	2.47	0.42
1:L:54:LEU:HB3	1:L:58:VAL:CG2	2.49	0.42
1:L:113:PRO:HB2	1:L:136:LEU:HD12	2.02	0.42
3:X:30:CYS:O	3:X:31:ALA:C	2.62	0.42
2:Q:29:PHE:CE2	2:Q:72:VAL:HG23	2.54	0.42
1:L:118:PHE:CD2	2:H:133:LEU:HB3	2.55	0.42
2:Q:51:ILE:HG13	2:Q:52:ASP:N	2.34	0.42
1:L:54:LEU:HD21	1:L:62:PHE:O	2.19	0.42
1:L:123:GLU:O	1:L:126:THR:HB	2.18	0.42
2:H:163:TRP:CD2	2:H:190:VAL:HG21	2.54	0.42
3:Y:103:ASN:N	3:Y:103:ASN:OD1	2.52	0.42
1:L:171:SER:O	1:L:172:THR:O	2.37	0.42
2:H:37:VAL:HG21	2:H:112:TRP:CZ3	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:30:SER:O	1:P:32:TYR:CD1	2.72	0.42
1:P:48:ILE:HG23	1:P:53:ARG:H	1.85	0.42
1:P:93:THR:HG22	1:P:94:LEU:H	1.85	0.42
1:P:146:VAL:CG2	1:P:161:ASN:HD21	2.32	0.42
2:Q:60:TYR:HE1	2:Q:70:LEU:HD23	1.85	0.42
2:Q:204:CYS:O	2:Q:204:CYS:SG	2.77	0.42
3:Y:9:ALA:HB1	3:Y:25:LEU:HD11	2.00	0.42
1:L:118:PHE:HA	1:L:119:PRO:HD3	1.87	0.42
1:L:162:SER:OG	2:H:176:PRO:HD2	2.20	0.42
2:H:140:GLN:O	2:H:141:THR:C	2.60	0.42
2:H:147:LEU:CG	2:H:219:ILE:HG21	2.48	0.42
3:X:6:CYS:O	3:X:7:GLU:C	2.63	0.42
1:P:78:LEU:O	1:P:78:LEU:HD22	2.20	0.42
3:Y:105:MET:HG3	3:Y:108:TRP:CE3	2.54	0.42
1:L:171:SER:OG	1:L:172:THR:N	2.52	0.42
2:H:33:TRP:CE3	2:H:50:GLU:HG2	2.54	0.42
2:H:64:PHE:O	2:H:66:GLY:N	2.52	0.42
2:H:86:LEU:HD23	2:H:86:LEU:HA	1.88	0.42
1:P:190:ASN:ND2	1:P:212:ASN:OD1	2.53	0.42
1:L:170:ASP:N	1:L:170:ASP:OD1	2.53	0.42
3:X:25:LEU:HA	3:X:25:LEU:HD23	1.83	0.42
1:P:209:PHE:CD1	1:P:209:PHE:C	2.97	0.42
2:Q:67:LYS:HD3	2:Q:67:LYS:N	2.35	0.42
1:L:113:PRO:CB	1:L:136:LEU:HD12	2.50	0.41
1:L:144:ILE:O	1:L:144:ILE:HG23	2.19	0.41
3:X:34:PHE:CD1	3:X:34:PHE:N	2.88	0.41
1:P:33:LEU:CD2	1:P:71:TYR:CG	3.03	0.41
3:Y:33:LYS:HG2	3:Y:38:PHE:CE1	2.55	0.41
3:Y:116:LYS:HD3	3:Y:116:LYS:N	2.34	0.41
1:L:136:LEU:C	1:L:137:ASN:HD22	2.27	0.41
1:L:138:ASN:OD1	2:H:173:HIS:HE1	2.03	0.41
2:H:133:LEU:HB2	2:H:148:GLY:O	2.20	0.41
3:Y:65:ASN:HB2	3:Y:74:ASN:ND2	2.35	0.41
3:Y:113:LYS:CA	3:Y:116:LYS:HD2	2.49	0.41
1:L:34:ASN:CG	2:H:108:VAL:HG22	2.44	0.41
1:L:150:ILE:HB	1:L:192:TYR:CE1	2.55	0.41
2:H:108:VAL:O	2:H:108:VAL:HG12	2.21	0.41
1:P:24:ARG:HG2	1:P:24:ARG:HH11	1.86	0.41
1:P:119:PRO:HG3	1:P:209:PHE:CG	2.55	0.41
1:P:119:PRO:HB3	1:P:209:PHE:CZ	2.55	0.41
1:P:174:SER:O	1:P:175:MET:HB3	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:164:ASN:HD21	2:Q:202:VAL:HA	1.84	0.41
1:L:124:GLN:HB2	2:H:131:TYR:CD2	2.55	0.41
2:H:57:TYR:HA	2:H:58:PRO:HD2	1.92	0.41
1:P:19:VAL:HG23	1:P:75:ILE:HB	2.03	0.41
2:Q:146:THR:C	2:Q:147:LEU:HD23	2.46	0.41
2:Q:193:PRO:O	2:Q:196:PRO:HD2	2.19	0.41
3:Y:128:ARG:HD2	3:Y:128:ARG:HA	1.77	0.41
1:L:110:ASP:HB3	1:L:200:THR:CG2	2.49	0.41
2:H:168:LEU:HD21	2:H:190:VAL:HG11	2.01	0.41
1:L:4:MET:HE1	1:L:33:LEU:HD21	2.01	0.41
1:L:105:GLU:HG3	1:L:166:GLN:NE2	2.36	0.41
2:H:11:LEU:HD13	2:H:119:THR:HB	2.02	0.41
3:Y:106:ASN:OD1	3:Y:106:ASN:N	2.53	0.41
1:L:39:LYS:HB3	1:L:40:PRO:HD2	2.01	0.41
1:L:136:LEU:N	1:L:136:LEU:HD22	2.36	0.41
2:H:37:VAL:CG2	2:H:112:TRP:CZ3	3.03	0.41
2:H:37:VAL:HG22	2:H:112:TRP:HZ3	1.84	0.41
3:X:34:PHE:CE1	3:X:123:TRP:CZ2	3.09	0.41
3:X:48:ASP:O	3:X:48:ASP:CG	2.63	0.41
3:X:61:ARG:HH11	3:X:61:ARG:CG	2.33	0.41
2:Q:38:LYS:HE3	2:Q:94:TYR:CZ	2.56	0.41
1:L:4:MET:HE1	1:L:33:LEU:CD2	2.51	0.41
1:L:119:PRO:HB3	1:L:209:PHE:CE1	2.56	0.41
1:L:186:TYR:HD1	1:L:192:TYR:CE2	2.38	0.41
2:H:88:SER:HA	2:H:120:VAL:CG2	2.51	0.41
2:H:175:PHE:O	2:H:186:LEU:CD1	2.69	0.41
3:X:4:GLY:H	3:X:7:GLU:HB3	1.85	0.41
3:X:63:TRP:CD1	3:X:63:TRP:H	2.38	0.41
3:X:80:CYS:O	3:X:81:SER:C	2.62	0.41
3:X:111:TRP:CZ3	3:X:116:LYS:HB2	2.55	0.41
2:Q:60:TYR:CE1	2:Q:70:LEU:HB2	2.53	0.41
2:H:172:VAL:O	2:H:173:HIS:CD2	2.74	0.41
3:X:3:PHE:O	3:X:38:PHE:HD2	2.03	0.41
3:X:8:LEU:HD21	3:X:32:ALA:CB	2.51	0.41
1:P:16:GLY:O	1:P:77:ASN:HA	2.21	0.41
1:P:49:TYR:CE2	1:P:53:ARG:HB3	2.56	0.41
2:H:10:GLU:CG	2:H:18:VAL:HG21	2.51	0.40
3:X:17:LEU:HD22	3:X:28:TRP:CD2	2.56	0.40
1:P:142:LYS:HD3	1:P:173:TYR:CG	2.56	0.40
1:L:169:LYS:NZ	1:L:169:LYS:HB2	2.36	0.40
2:H:27:TYR:CD1	2:H:27:TYR:C	2.99	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:130:VAL:C	2:H:131:TYR:CD1	2.99	0.40
2:H:216:ASP:N	2:H:216:ASP:OD1	2.53	0.40
3:X:27:ASN:O	3:X:31:ALA:HB2	2.21	0.40
1:P:50:TYR:CD1	2:Q:106:TYR:HE1	2.39	0.40
1:P:160:LEU:HD11	2:Q:180:GLN:HG3	2.03	0.40
1:L:33:LEU:HD22	1:L:89:GLN:O	2.22	0.40
2:H:193:PRO:HB2	2:H:196:PRO:CD	2.51	0.40
3:Y:45:ARG:H	3:Y:45:ARG:HH11	1.68	0.40
2:H:87:THR:O	2:H:88:SER:C	2.65	0.40
2:H:147:LEU:HD11	2:H:197:ARG:HD3	2.04	0.40
3:X:101:ASP:O	3:X:101:ASP:CG	2.63	0.40
1:L:160:LEU:N	1:L:178:THR:O	2.55	0.40
1:P:201:SER:O	1:P:202:THR:HB	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	L	212/214 (99%)	167 (79%)	31 (15%)	14 (7%)	1	5
1	P	212/214 (99%)	168 (79%)	35 (16%)	9 (4%)	2	13
2	H	219/221 (99%)	186 (85%)	20 (9%)	13 (6%)	1	7
2	Q	219/221 (99%)	179 (82%)	30 (14%)	10 (5%)	2	11
3	X	127/129 (98%)	97 (76%)	23 (18%)	7 (6%)	1	8
3	Y	127/129 (98%)	93 (73%)	26 (20%)	8 (6%)	1	6
All	All	1116/1128 (99%)	890 (80%)	165 (15%)	61 (6%)	1	8

All (61) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	15	LEU
1	L	80	GLN
1	L	110	ASP
1	L	171	SER
1	L	172	THR
1	L	199	LYS
2	H	140	GLN
2	H	169	SER
2	H	210	ALA
3	X	48	ASP
3	X	104	GLY
1	P	165	ASP
1	P	185	GLU
2	Q	65	LYS
2	Q	114	GLN
2	Q	135	PRO
2	Q	156	PRO
3	Y	18	ASP
1	L	67	SER
1	L	169	LYS
1	L	178	THR
1	L	188	ARG
2	H	65	LYS
2	H	138	ALA
2	H	199	SER
3	X	49	GLY
1	P	138	ASN
1	P	151	ASP
1	P	200	THR
2	Q	7	PRO
2	Q	30	THR
3	Y	86	SER
3	Y	103	ASN
3	Y	109	VAL
2	H	177	ALA
2	H	201	THR
3	X	62	TRP
1	P	41	ASP
2	Q	137	SER
2	Q	199	SER
3	Y	61	ARG
3	Y	111	TRP
1	L	116	SER

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Mol	Chain	Res	Type
1	L	157	ASN
2	H	104	THR
2	H	141	THR
1	P	40	PRO
2	Q	41	PRO
3	Y	41	GLN
3	X	5	ARG
3	X	61	ARG
3	X	68	ARG
1	P	68	GLY
1	L	30	SER
1	L	162	SER
2	H	2	VAL
1	P	186	TYR
2	H	171	GLY
3	Y	67	GLY
2	H	151	VAL
2	Q	8	GLY

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	P	186/192 (97%)	171 (92%)	15 (8%)	11	38
2	H	48/190 (25%)	43 (90%)	5 (10%)	7	28
2	Q	174/190 (92%)	154 (88%)	20 (12%)	5	24
3	X	105/105 (100%)	93 (89%)	12 (11%)	5	24
3	Y	104/105 (99%)	93 (89%)	11 (11%)	6	27
All	All	617/782 (79%)	554 (90%)	63 (10%)	7	29

All (63) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	H	178	VAL

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Mol	Chain	Res	Type
2	H	195	SER
2	H	199	SER
2	H	203	THR
2	H	216	ASP
3	X	2	VAL
3	X	25	LEU
3	X	30	CYS
3	X	38	PHE
3	X	50	SER
3	X	61	ARG
3	X	62	TRP
3	X	81	SER
3	X	86	SER
3	X	91	THR
3	X	98	ILE
3	X	105	MET
1	P	7	THR
1	P	34	ASN
1	P	46	LEU
1	P	74	THR
1	P	78	LEU
1	P	93	THR
1	P	94	LEU
1	P	98	PHE
1	P	106	ILE
1	P	117	ILE
1	P	169	LYS
1	P	171	SER
1	P	207	LYS
1	P	209	PHE
1	P	213	GLU
2	Q	12	VAL
2	Q	30	THR
2	Q	59	ASN
2	Q	78	THR
2	Q	96	CYS
2	Q	99	LEU
2	Q	108	VAL
2	Q	114	GLN
2	Q	125	THR
2	Q	130	VAL
2	Q	133	LEU

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Mol	Chain	Res	Type
2	Q	147	LEU
2	Q	157	GLU
2	Q	160	THR
2	Q	179	LEU
2	Q	199	SER
2	Q	203	THR
2	Q	205	ASN
2	Q	212	SER
2	Q	217	LYS
3	Y	33	LYS
3	Y	44	ASN
3	Y	45	ARG
3	Y	47	THR
3	Y	62	TRP
3	Y	86	SER
3	Y	103	ASN
3	Y	106	ASN
3	Y	108	TRP
3	Y	109	VAL
3	Y	116	LYS

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

Mol	Chain	Res	Type
2	H	205	ASN
2	H	208	HIS
3	X	37	ASN
3	X	57	GLN
3	X	84	GLN
3	X	103	ASN
3	X	114	HIS
1	P	55	HIS
1	P	89	GLN
1	P	166	GLN
2	Q	35	HIS
2	Q	82	GLN
2	Q	140	GLN
2	Q	164	ASN
3	Y	27	ASN
3	Y	57	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.