



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 10:48 AM UTC

PDB ID : 1HYN / pdb_00001hyn
Title : CRYSTAL STRUCTURE OF THE CYTOPLASMIC DOMAIN OF HUMAN
ERYTHROCYTE BAND-3 PROTEIN
Authors : Zhang, D.; Kiyatkin, A.; Bolin, J.T.; Low, P.S.
Deposited on : 2001-01-20
Resolution : 2.60 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
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

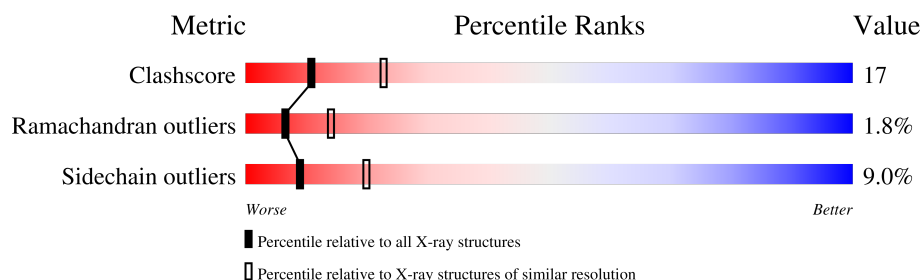
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	P	379	
1	Q	379	
1	R	379	
1	S	379	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 9698 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 BAND 3 ANION TRANSPORT PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	P	293	Total	C	N	O	S	0	0	0
			2318	1473	404	435	6			
1	Q	302	Total	C	N	O	S	0	0	0
			2382	1511	416	449	6			
1	R	300	Total	C	N	O	S	0	0	0
			2366	1502	412	446	6			
1	S	293	Total	C	N	O	S	0	0	0
			2318	1473	404	435	6			

- Molecule 2 is water.

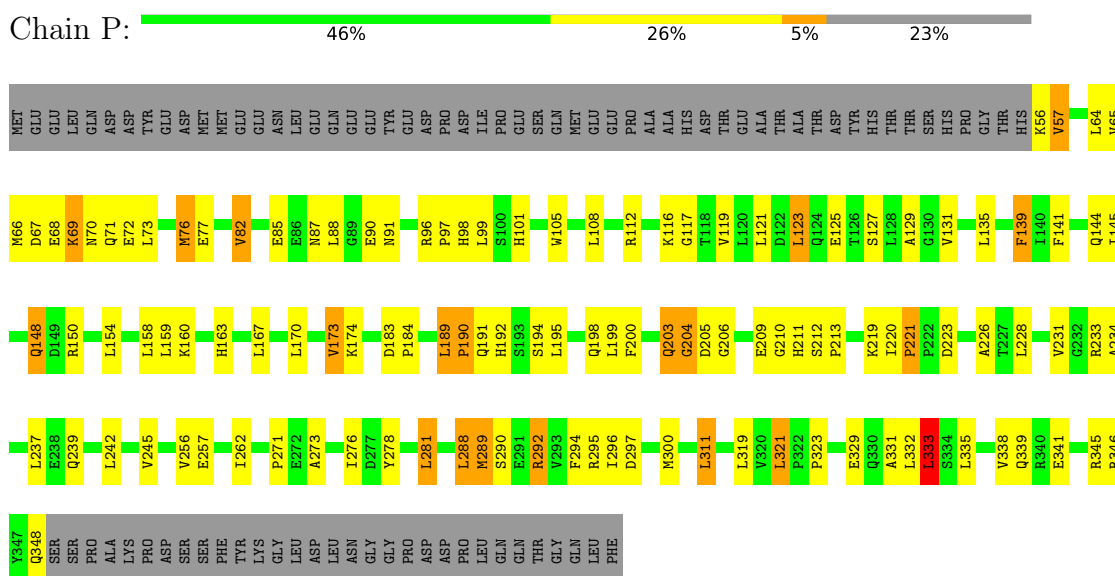
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	P	71	Total	O	0	0
			71	71		
2	Q	87	Total	O	0	0
			87	87		
2	R	87	Total	O	0	0
			87	87		
2	S	69	Total	O	0	0
			69	69		

3 Residue-property plots

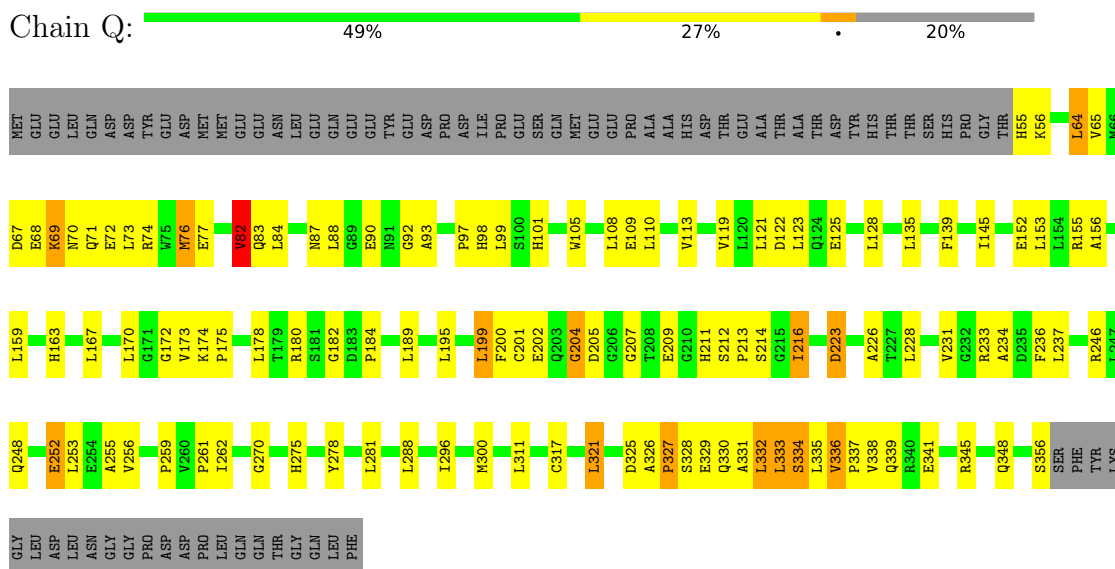
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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.

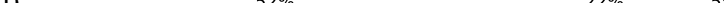
- Molecule 1: BAND 3 ANION TRANSPORT PROTEIN

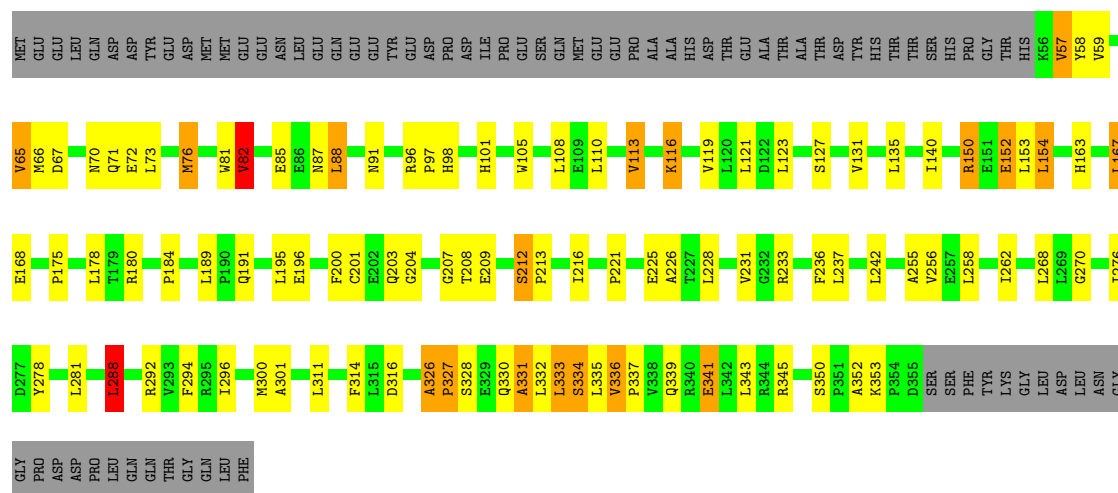


- Molecule 1: BAND 3 ANION TRANSPORT PROTEIN

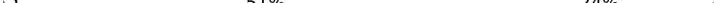


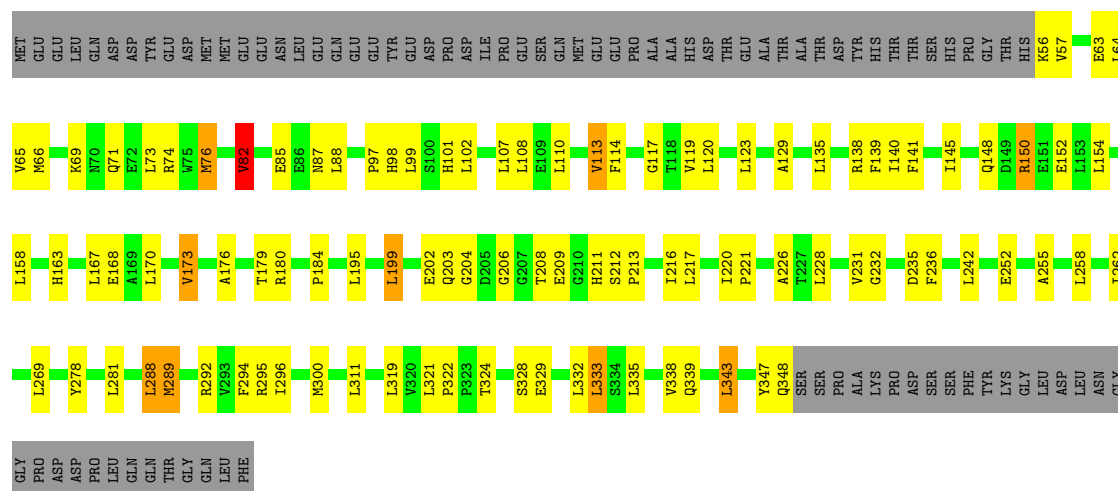
• Molecule 1: BAND 3 ANION TRANSPORT PROTEIN

Chain R:  52% 22% 5% • 21%



• Molecule 1: BAND 3 ANION TRANSPORT PROTEIN

Chain S:  51% 24% 1% 23%



4 Data and refinement statistics

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

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	181.59Å 92.58Å 123.33Å 90.00° 131.86° 90.00°	Depositor
Resolution (Å)	8.00 – 2.60	Depositor
% Data completeness (in resolution range)	99.0 (8.00-2.60)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.216 , 0.290	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	9698	wwPDB-VP
Average B, all atoms (Å ²)	31.0	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	P	0.55	2/2366 (0.1%)	1.04	19/3213 (0.6%)
1	Q	0.53	1/2433 (0.0%)	1.02	8/3305 (0.2%)
1	R	0.53	1/2416 (0.0%)	1.09	21/3282 (0.6%)
1	S	0.55	2/2366 (0.1%)	1.03	13/3213 (0.4%)
All	All	0.54	6/9581 (0.1%)	1.04	61/13013 (0.5%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	S	76	MET	SD-CE	-7.75	1.60	1.79
1	R	76	MET	SD-CE	-7.65	1.60	1.79
1	S	289	MET	SD-CE	-6.96	1.62	1.79
1	P	76	MET	SD-CE	-6.58	1.63	1.79
1	Q	76	MET	SD-CE	-6.14	1.64	1.79
1	P	289	MET	SD-CE	-5.13	1.66	1.79

All (61) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	R	334	SER	N-CA-C	-10.21	100.56	113.43
1	Q	334	SER	N-CA-C	-9.17	101.99	113.55
1	S	117	GLY	N-CA-C	8.80	122.05	111.93
1	S	71	GLN	O-C-N	7.91	131.89	122.00
1	P	204	GLY	N-CA-C	-7.57	104.42	114.25
1	Q	201	CYS	N-CA-C	7.27	119.84	111.11
1	S	220	ILE	CA-C-N	7.21	124.92	119.66
1	S	220	ILE	C-N-CA	7.21	124.92	119.66
1	R	331	ALA	N-CA-C	-7.11	103.14	111.03
1	R	82	VAL	N-CA-C	-6.99	94.81	109.34
1	P	333	LEU	N-CA-C	-6.92	104.65	113.23
1	S	221	PRO	N-CA-C	6.84	117.04	110.47
1	P	203	GLN	N-CA-C	6.73	119.58	108.48
1	R	201	CYS	N-CA-C	6.65	121.48	113.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Q	326	ALA	N-CA-C	6.63	124.46	109.81
1	P	82	VAL	N-CA-C	-6.58	95.64	109.34
1	S	150	ARG	N-CA-C	6.51	118.03	111.07
1	S	221	PRO	CA-C-N	6.40	127.84	119.84
1	S	221	PRO	C-N-CA	6.40	127.84	119.84
1	P	221	PRO	N-CA-C	6.36	118.46	110.70
1	P	220	ILE	CA-C-N	6.31	126.88	120.38
1	P	220	ILE	C-N-CA	6.31	126.88	120.38
1	Q	82	VAL	N-CA-C	-6.30	96.24	109.34
1	R	326	ALA	N-CA-C	6.12	118.39	109.71
1	R	150	ARG	N-CA-C	6.05	118.37	111.11
1	S	82	VAL	N-CA-C	-6.02	96.81	109.34
1	R	221	PRO	CA-C-N	5.89	127.20	119.84
1	R	221	PRO	C-N-CA	5.89	127.20	119.84
1	S	56	LYS	N-CA-C	-5.86	94.60	111.00
1	P	221	PRO	CA-C-N	5.78	126.17	119.47
1	P	221	PRO	C-N-CA	5.78	126.17	119.47
1	Q	248	GLN	N-CA-C	-5.76	105.00	111.28
1	R	288	LEU	N-CA-C	-5.74	104.93	111.07
1	P	189	LEU	CA-C-N	5.72	126.99	119.84
1	P	189	LEU	C-N-CA	5.72	126.99	119.84
1	R	276	ILE	N-CA-C	5.69	115.53	106.88
1	R	301	ALA	N-CA-C	5.67	118.45	110.23
1	S	333	LEU	N-CA-C	-5.64	105.66	112.54
1	R	326	ALA	CA-C-N	5.58	126.81	119.84
1	R	326	ALA	C-N-CA	5.58	126.81	119.84
1	Q	332	LEU	N-CA-C	5.54	118.03	111.33
1	P	297	ASP	N-CA-C	-5.53	105.27	112.23
1	S	281	LEU	N-CA-C	-5.47	105.39	111.36
1	R	116	LYS	N-CA-C	-5.45	105.94	112.59
1	Q	348	GLN	N-CA-C	5.41	116.86	111.07
1	P	150	ARG	N-CA-C	5.41	117.60	111.11
1	R	105	TRP	N-CA-C	5.39	117.23	111.36
1	S	101	HIS	N-CA-C	-5.37	101.78	110.32
1	R	353	LYS	CA-C-N	5.31	125.25	119.78
1	R	353	LYS	C-N-CA	5.31	125.25	119.78
1	P	281	LEU	N-CA-C	-5.31	105.49	111.28
1	R	292	ARG	N-CA-C	5.28	117.47	111.02
1	P	101	HIS	N-CA-C	-5.25	101.97	110.32
1	P	292	ARG	N-CA-C	5.25	117.42	111.02
1	P	105	TRP	N-CA-C	5.24	116.67	111.07
1	Q	64	LEU	N-CA-C	-5.21	101.93	109.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	P	117	GLY	N-CA-C	5.18	119.17	112.54
1	R	101	HIS	N-CA-C	-5.14	100.52	108.90
1	R	58	TYR	N-CA-C	-5.07	101.69	109.76
1	P	311	LEU	N-CA-C	-5.02	105.81	111.28
1	R	200	PHE	N-CA-C	5.02	121.10	114.12

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	P	2318	0	2320	103	0
1	Q	2382	0	2378	105	0
1	R	2366	0	2366	83	0
1	S	2318	0	2320	84	0
2	P	71	0	0	3	0
2	Q	87	0	0	4	0
2	R	87	0	0	3	0
2	S	69	0	0	0	0
All	All	9698	0	9384	312	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 17.

All (312) 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:S:73:LEU:HD13	1:S:184:PRO:HB3	1.29	1.11
1:R:73:LEU:HD13	1:R:184:PRO:HB3	1.30	1.08
1:Q:73:LEU:HD13	1:Q:184:PRO:HB3	1.36	1.07
1:S:87:ASN:HD21	1:S:98:HIS:HE1	1.12	0.98
1:P:73:LEU:O	1:P:159:LEU:HD13	1.66	0.95
1:P:332:LEU:HD22	1:Q:335:LEU:HD22	1.52	0.90
1:P:332:LEU:HB3	1:Q:335:LEU:HB3	1.55	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:296:ILE:HG22	1:S:300:MET:HE2	1.55	0.86
1:Q:256:VAL:HG21	1:Q:262:ILE:HD11	1.57	0.84
1:R:333:LEU:HD21	1:S:99:LEU:H	1.42	0.84
1:R:330:GLN:O	1:R:333:LEU:HD22	1.77	0.84
1:P:73:LEU:HD13	1:P:184:PRO:HB3	1.58	0.84
1:P:341:GLU:HG2	1:Q:195:LEU:HD13	1.59	0.84
1:R:73:LEU:HD13	1:R:184:PRO:CB	2.10	0.80
1:Q:331:ALA:HB1	1:Q:335:LEU:HD12	1.63	0.80
1:Q:325:ASP:O	1:Q:327:PRO:HD3	1.81	0.79
1:R:335:LEU:HB3	1:S:332:LEU:HB3	1.65	0.79
1:P:333:LEU:HD13	1:Q:332:LEU:HD21	1.69	0.75
1:R:335:LEU:HB3	1:S:332:LEU:HD22	1.67	0.74
1:Q:87:ASN:HD21	1:Q:98:HIS:HE1	1.36	0.74
1:S:208:THR:HB	1:S:212:SER:HB3	1.69	0.73
1:R:335:LEU:O	1:S:332:LEU:HD13	1.89	0.73
1:Q:180:ARG:HG3	1:Q:236:PHE:HB3	1.71	0.72
1:S:87:ASN:ND2	1:S:98:HIS:HE1	1.88	0.72
1:Q:333:LEU:HD23	1:Q:334:SER:N	2.04	0.72
1:Q:333:LEU:HD23	1:Q:334:SER:H	1.55	0.71
1:S:343:LEU:HD22	1:S:347:TYR:HE1	1.56	0.71
1:P:332:LEU:CB	1:Q:335:LEU:HB3	2.20	0.69
1:Q:76:MET:HE1	1:Q:163:HIS:C	2.18	0.69
1:P:76:MET:HE1	1:P:163:HIS:C	2.18	0.68
1:R:195:LEU:HD21	1:S:338:VAL:HG13	1.75	0.68
1:R:333:LEU:HD21	1:S:99:LEU:N	2.07	0.68
1:Q:226:ALA:HB3	1:Q:262:ILE:HD13	1.75	0.67
1:R:327:PRO:HB2	1:R:330:GLN:HB2	1.77	0.67
1:S:289:MET:CE	1:S:295:ARG:HG3	2.24	0.67
1:P:209:GLU:HB2	1:P:212:SER:OG	1.95	0.67
1:R:335:LEU:C	1:S:332:LEU:HD13	2.20	0.67
1:P:199:LEU:HD12	1:Q:337:PRO:HB2	1.75	0.67
1:R:339:GLN:HG3	1:S:332:LEU:HD11	1.77	0.66
1:P:256:VAL:HG21	1:P:262:ILE:HD11	1.77	0.66
1:S:226:ALA:HB3	1:S:262:ILE:HD13	1.77	0.66
1:R:87:ASN:HD21	1:R:98:HIS:HE1	1.42	0.66
1:S:87:ASN:HD21	1:S:98:HIS:CE1	2.04	0.66
1:S:163:HIS:HE1	1:S:255:ALA:O	1.78	0.65
1:R:127:SER:O	1:R:131:VAL:HG23	1.96	0.65
1:R:333:LEU:HD23	1:R:334:SER:N	2.11	0.65
1:R:191:GLN:HA	1:R:191:GLN:OE1	1.97	0.65
1:P:98:HIS:HA	1:Q:333:LEU:HG	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:195:LEU:HG	1:Q:345:ARG:HH21	1.62	0.65
1:R:88:LEU:HD13	1:R:167:LEU:HD12	1.79	0.65
1:R:335:LEU:HB3	1:S:332:LEU:CB	2.27	0.65
1:S:180:ARG:HG2	1:S:236:PHE:HB3	1.79	0.64
1:S:329:GLU:O	1:S:333:LEU:HB2	1.97	0.64
1:R:333:LEU:HD11	1:S:98:HIS:HA	1.79	0.64
1:S:296:ILE:HG22	1:S:300:MET:CE	2.27	0.63
1:Q:70:ASN:ND2	1:Q:72:GLU:HG3	2.12	0.63
1:S:76:MET:HE1	1:S:163:HIS:C	2.23	0.63
1:P:123:LEU:HD22	1:P:125:GLU:HG2	1.80	0.62
1:Q:252:GLU:HB3	2:Q:5859:HOH:O	1.98	0.62
1:R:332:LEU:HD21	1:S:333:LEU:HD13	1.80	0.62
1:S:66:MET:HB2	1:S:176:ALA:HB2	1.81	0.62
1:Q:189:LEU:HD11	1:S:141:PHE:CZ	2.35	0.62
1:R:296:ILE:O	1:R:300:MET:HG3	1.99	0.62
1:P:341:GLU:HG2	1:Q:195:LEU:CD1	2.30	0.61
1:S:343:LEU:HD22	1:S:347:TYR:CE1	2.35	0.61
1:Q:84:LEU:HB2	1:Q:216:ILE:HD11	1.82	0.61
1:Q:231:VAL:CG1	1:Q:278:TYR:HB3	2.30	0.61
1:S:85:GLU:O	1:S:97:PRO:HA	2.00	0.61
1:P:233:ARG:NH1	1:P:278:TYR:HB2	2.15	0.60
1:P:99:LEU:HB2	1:Q:333:LEU:HD21	1.83	0.60
1:Q:345:ARG:HH11	1:Q:345:ARG:HG2	1.66	0.60
1:P:87:ASN:OD1	1:P:98:HIS:HE1	1.85	0.60
1:R:59:VAL:HB	1:R:81:TRP:HB2	1.84	0.59
1:P:332:LEU:HD13	1:Q:335:LEU:C	2.27	0.59
1:P:73:LEU:O	1:P:159:LEU:CD1	2.47	0.59
1:Q:296:ILE:O	1:Q:300:MET:HG3	2.03	0.59
1:P:141:PHE:CE1	1:R:189:LEU:HD11	2.39	0.58
1:P:141:PHE:CE2	1:R:189:LEU:HD21	2.39	0.58
1:R:140:ILE:HD11	1:R:150:ARG:HB2	1.86	0.58
1:P:345:ARG:O	1:P:348:GLN:HG2	2.03	0.58
1:Q:69:LYS:HG3	1:Q:70:ASN:H	1.69	0.58
1:Q:87:ASN:HD21	1:Q:98:HIS:CE1	2.20	0.57
1:P:296:ILE:O	1:P:300:MET:HG3	2.04	0.57
1:R:231:VAL:CG1	1:R:278:TYR:HB3	2.35	0.57
1:R:339:GLN:CG	1:S:332:LEU:HD11	2.35	0.57
1:P:141:PHE:CZ	1:R:189:LEU:HD11	2.40	0.57
1:Q:139:PHE:HB3	1:Q:145:ILE:HG12	1.87	0.57
1:P:127:SER:O	1:P:131:VAL:HG23	2.05	0.57
1:P:76:MET:HE3	1:P:77:GLU:H	1.69	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:332:LEU:HD13	1:Q:335:LEU:CA	2.35	0.56
1:R:73:LEU:CD1	1:R:184:PRO:HB3	2.20	0.56
1:P:99:LEU:HD13	1:Q:321:LEU:HD21	1.88	0.56
1:Q:209:GLU:HB3	1:Q:212:SER:HB2	1.87	0.56
1:P:148:GLN:HG3	2:P:5942:HOH:O	2.06	0.55
1:R:335:LEU:HB3	1:S:332:LEU:CD2	2.36	0.55
1:R:335:LEU:CB	1:S:332:LEU:HD22	2.36	0.55
1:S:179:THR:HA	1:S:235:ASP:OD2	2.07	0.55
1:S:57:VAL:HG21	1:S:295:ARG:HD3	1.88	0.55
1:R:242:LEU:HD12	1:R:268:LEU:HD21	1.88	0.55
1:S:163:HIS:CE1	1:S:255:ALA:O	2.60	0.55
1:Q:90:GLU:O	1:Q:167:LEU:HD21	2.06	0.55
1:P:65:VAL:CG2	1:P:173:VAL:HG21	2.37	0.55
1:R:296:ILE:HG22	1:R:300:MET:HE2	1.89	0.55
1:Q:73:LEU:HD13	1:Q:184:PRO:CB	2.24	0.54
1:Q:212:SER:N	1:Q:213:PRO:HD2	2.23	0.54
1:R:233:ARG:HA	1:R:270:GLY:O	2.08	0.54
1:P:66:MET:HA	1:P:72:GLU:O	2.07	0.54
1:R:152:GLU:HB2	2:R:5950:HOH:O	2.07	0.54
1:P:234:ALA:HB3	1:P:237:LEU:HD12	1.89	0.54
1:P:292:ARG:HG3	1:P:292:ARG:HH11	1.72	0.54
1:Q:261:PRO:HG3	2:Q:5859:HOH:O	2.07	0.54
1:S:82:VAL:HB	1:S:216:ILE:HG12	1.90	0.54
1:Q:70:ASN:HD22	1:Q:72:GLU:HG3	1.73	0.53
1:R:57:VAL:HA	1:R:225:GLU:O	2.08	0.53
1:R:119:VAL:HG12	1:R:121:LEU:HG	1.90	0.53
1:S:288:LEU:HD22	1:S:294:PHE:CG	2.43	0.53
1:S:195:LEU:HD22	1:S:199:LEU:CD2	2.37	0.53
1:S:57:VAL:CG2	1:S:295:ARG:HD3	2.39	0.53
1:P:73:LEU:C	1:P:159:LEU:HD13	2.33	0.53
1:P:116:LYS:NZ	1:P:239:GLN:HE22	2.05	0.53
1:S:179:THR:HG22	1:S:180:ARG:N	2.24	0.53
1:Q:76:MET:HE3	1:Q:77:GLU:N	2.23	0.53
1:Q:87:ASN:ND2	1:Q:98:HIS:HE1	2.04	0.53
1:P:139:PHE:HB3	1:P:145:ILE:HG12	1.89	0.52
1:P:199:LEU:HD21	1:Q:341:GLU:HG3	1.91	0.52
1:S:209:GLU:HB2	1:S:212:SER:HB2	1.91	0.52
1:R:226:ALA:HB3	1:R:262:ILE:HD13	1.90	0.52
1:R:345:ARG:HG2	1:R:345:ARG:HH11	1.75	0.52
1:R:341:GLU:HG3	1:S:199:LEU:HD21	1.92	0.52
1:S:73:LEU:HD13	1:S:184:PRO:CB	2.20	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:90:GLU:O	1:P:167:LEU:HD11	2.10	0.52
1:P:226:ALA:HB3	1:P:262:ILE:HD13	1.92	0.52
1:P:99:LEU:H	1:Q:333:LEU:HD21	1.74	0.52
1:Q:296:ILE:HG22	1:Q:300:MET:HE2	1.91	0.52
1:Q:109:GLU:O	1:Q:113:VAL:HG22	2.09	0.52
1:R:180:ARG:HG3	1:R:236:PHE:HB3	1.92	0.52
1:R:331:ALA:HB1	1:R:335:LEU:HD12	1.91	0.52
1:S:98:HIS:HD2	1:S:99:LEU:O	1.92	0.52
1:R:212:SER:N	1:R:213:PRO:HD2	2.25	0.52
1:Q:97:PRO:HB3	1:Q:216:ILE:HD12	1.92	0.51
1:P:289:MET:HE1	1:P:295:ARG:HA	1.93	0.51
1:Q:93:ALA:CB	1:Q:204:GLY:HA3	2.41	0.51
1:R:85:GLU:O	1:R:97:PRO:HA	2.10	0.51
1:R:256:VAL:HG21	1:R:262:ILE:HD11	1.92	0.51
1:R:333:LEU:HD23	1:R:333:LEU:C	2.35	0.51
1:P:65:VAL:HG21	1:P:173:VAL:HG21	1.93	0.51
1:P:68:GLU:HG2	1:P:174:LYS:HG3	1.93	0.51
1:P:129:ALA:HA	1:P:158:LEU:HD21	1.93	0.51
1:R:163:HIS:HE1	1:R:255:ALA:O	1.93	0.50
1:P:233:ARG:HH11	1:P:278:TYR:HB2	1.75	0.50
1:Q:105:TRP:CE3	1:Q:275:HIS:HB3	2.46	0.50
1:S:139:PHE:HB3	1:S:145:ILE:HG12	1.93	0.50
1:P:332:LEU:HD11	1:Q:339:GLN:HB2	1.92	0.50
1:R:76:MET:HE1	1:R:163:HIS:C	2.37	0.50
1:R:314:PHE:CZ	1:S:322:PRO:HB3	2.46	0.50
1:P:69:LYS:HB2	1:P:170:LEU:O	2.12	0.50
1:P:98:HIS:CA	1:Q:333:LEU:HG	2.40	0.50
1:Q:82:VAL:O	1:Q:83:GLN:HB2	2.12	0.49
1:R:175:PRO:HB3	1:R:191:GLN:HE21	1.76	0.49
1:P:108:LEU:O	1:P:112:ARG:HG3	2.13	0.49
1:P:273:ALA:HB3	1:P:276:ILE:CG2	2.42	0.49
1:P:332:LEU:HD13	1:Q:335:LEU:HA	1.95	0.49
1:P:323:PRO:HG3	1:Q:317:CYS:HB2	1.95	0.49
1:R:65:VAL:O	1:R:73:LEU:HD12	2.13	0.49
1:S:119:VAL:O	1:S:120:LEU:HD23	2.12	0.49
1:Q:178:LEU:HD11	1:Q:182:GLY:HA2	1.94	0.49
1:P:148:GLN:H	1:P:148:GLN:NE2	2.10	0.49
1:S:292:ARG:HD2	1:S:347:TYR:HE2	1.77	0.48
1:Q:92:GLY:HA2	1:Q:167:LEU:HD13	1.94	0.48
1:Q:93:ALA:HB1	1:Q:204:GLY:HA3	1.96	0.48
1:Q:189:LEU:HD11	1:S:141:PHE:CE1	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:212:SER:N	1:S:213:PRO:CD	2.77	0.48
1:Q:67:ASP:HA	1:Q:173:VAL:HA	1.94	0.48
1:Q:174:LYS:HD2	1:Q:175:PRO:HD2	1.96	0.48
1:S:292:ARG:HG3	1:S:292:ARG:HH11	1.79	0.48
1:S:65:VAL:O	1:S:73:LEU:HD12	2.13	0.48
1:P:73:LEU:O	1:P:159:LEU:HD22	2.14	0.48
1:P:91:ASN:HD21	1:P:204:GLY:HA2	1.78	0.48
1:R:335:LEU:O	1:R:336:VAL:HG23	2.13	0.48
1:Q:180:ARG:H	1:Q:180:ARG:HD2	1.77	0.48
1:R:96:ARG:HG2	1:R:203:GLN:HE22	1.79	0.48
1:R:180:ARG:HG2	1:R:180:ARG:HH11	1.78	0.48
1:P:206:GLY:N	1:P:210:GLY:HA2	2.29	0.47
1:P:333:LEU:CD1	1:Q:332:LEU:HD21	2.43	0.47
1:Q:334:SER:O	1:Q:338:VAL:HB	2.14	0.47
1:R:82:VAL:HB	1:R:216:ILE:HG12	1.97	0.47
1:R:91:ASN:O	1:R:168:GLU:HG2	2.14	0.47
1:R:108:LEU:HD13	1:S:108:LEU:HD13	1.96	0.47
1:S:319:LEU:HD21	1:S:335:LEU:HD22	1.95	0.47
1:P:288:LEU:HD22	1:P:294:PHE:CG	2.49	0.47
1:R:196:GLU:CD	1:R:196:GLU:H	2.23	0.47
1:Q:69:LYS:HG2	1:Q:170:LEU:O	2.15	0.47
1:Q:341:GLU:O	1:Q:345:ARG:HG3	2.15	0.47
1:S:74:ARG:HG2	1:S:74:ARG:HH11	1.78	0.47
1:S:208:THR:HB	1:S:212:SER:CB	2.42	0.47
1:S:231:VAL:HG13	1:S:278:TYR:HB3	1.95	0.47
1:R:70:ASN:HB3	1:R:72:GLU:HG3	1.96	0.47
1:P:338:VAL:HA	1:Q:199:LEU:HD21	1.97	0.47
1:P:119:VAL:HG12	1:P:121:LEU:HG	1.96	0.47
1:P:231:VAL:HG13	1:P:278:TYR:HB3	1.96	0.47
1:Q:163:HIS:HE1	1:Q:255:ALA:O	1.98	0.47
1:R:87:ASN:ND2	1:R:98:HIS:HE1	2.10	0.46
1:Q:199:LEU:HD13	1:Q:200:PHE:CE1	2.51	0.46
1:P:67:ASP:OD1	1:P:72:GLU:HG3	2.16	0.46
1:R:258:LEU:HB3	2:R:6068:HOH:O	2.14	0.46
1:S:232:GLY:O	1:S:269:LEU:HA	2.15	0.46
1:P:73:LEU:CD1	1:P:184:PRO:HB3	2.39	0.46
1:P:338:VAL:HG21	1:Q:101:HIS:ND1	2.31	0.46
1:Q:55:HIS:HD2	1:Q:223:ASP:O	1.98	0.46
1:P:116:LYS:HZ2	1:P:239:GLN:HE22	1.63	0.46
1:P:289:MET:CE	1:P:295:ARG:HG3	2.45	0.46
1:Q:180:ARG:HG2	1:Q:180:ARG:HH11	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:141:PHE:CD2	1:R:189:LEU:HD21	2.50	0.46
1:S:203:GLN:HB2	1:S:206:GLY:O	2.15	0.46
1:R:207:GLY:C	1:R:209:GLU:H	2.23	0.45
1:S:113:VAL:HG13	1:S:242:LEU:HB2	1.97	0.45
1:Q:167:LEU:C	1:Q:167:LEU:HD23	2.41	0.45
1:Q:207:GLY:C	1:Q:209:GLU:H	2.25	0.45
1:Q:231:VAL:HG11	1:Q:278:TYR:HB3	1.97	0.45
1:S:99:LEU:HD23	1:S:99:LEU:HA	1.78	0.45
1:S:328:SER:O	1:S:332:LEU:HD12	2.17	0.45
1:P:139:PHE:O	1:P:144:GLN:HB2	2.16	0.45
1:P:332:LEU:HD11	1:Q:339:GLN:HG3	1.97	0.45
1:S:120:LEU:HD21	1:S:138:ARG:HG2	1.99	0.45
1:P:237:LEU:O	1:P:271:PRO:HB3	2.17	0.45
1:R:333:LEU:CD1	1:S:98:HIS:HA	2.46	0.45
1:S:343:LEU:CD2	1:S:347:TYR:HE1	2.25	0.45
1:R:116:LYS:HE3	2:R:5834:HOH:O	2.17	0.44
1:P:329:GLU:O	1:P:333:LEU:HB2	2.17	0.44
1:Q:156:ALA:HA	1:Q:159:LEU:HG	1.98	0.44
1:S:63:GLU:HG2	1:S:231:VAL:HB	1.98	0.44
1:P:96:ARG:HD2	1:P:200:PHE:HD2	1.81	0.44
1:P:99:LEU:HD12	1:Q:331:ALA:HA	1.98	0.44
1:R:96:ARG:HE	1:R:203:GLN:HE22	1.66	0.44
1:S:226:ALA:HB3	1:S:262:ILE:CD1	2.44	0.44
1:P:68:GLU:O	1:P:71:GLN:NE2	2.50	0.44
1:P:98:HIS:HA	1:Q:333:LEU:CG	2.45	0.44
1:P:123:LEU:HD12	1:P:245:VAL:HG11	2.00	0.44
1:P:319:LEU:HD22	1:P:335:LEU:HD13	1.99	0.44
1:Q:336:VAL:HB	1:Q:337:PRO:CD	2.48	0.44
1:R:336:VAL:HB	1:R:337:PRO:CD	2.47	0.44
1:P:99:LEU:HG	1:Q:330:GLN:O	2.18	0.43
1:Q:122:ASP:N	1:Q:246:ARG:O	2.51	0.43
1:R:66:MET:HA	1:R:72:GLU:O	2.18	0.43
1:Q:98:HIS:HD2	1:Q:99:LEU:O	2.02	0.43
1:R:113:VAL:HG13	1:R:242:LEU:HB2	2.00	0.43
1:R:153:LEU:HD11	1:R:237:LEU:HD21	1.99	0.43
1:P:57:VAL:HG21	1:P:295:ARG:HD3	2.00	0.43
1:P:85:GLU:O	1:P:97:PRO:HA	2.18	0.43
1:P:194:SER:O	1:P:198:GLN:HG3	2.18	0.43
1:P:219:LYS:O	1:P:221:PRO:HD3	2.19	0.43
1:R:330:GLN:HA	1:R:333:LEU:HD13	2.01	0.43
1:S:129:ALA:HA	1:S:158:LEU:HD21	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:119:VAL:HG12	1:Q:121:LEU:HG	2.01	0.43
1:Q:123:LEU:HG	1:Q:125:GLU:HG2	2.00	0.43
1:Q:300:MET:HG2	2:Q:5897:HOH:O	2.19	0.43
1:S:195:LEU:HD22	1:S:199:LEU:HD21	2.00	0.43
1:Q:74:ARG:HG2	1:Q:74:ARG:HH11	1.83	0.43
1:P:76:MET:HE3	1:P:77:GLU:N	2.34	0.43
1:Q:189:LEU:HD21	1:S:141:PHE:CD2	2.54	0.42
1:S:102:LEU:CD1	1:S:107:LEU:HD21	2.49	0.42
1:P:332:LEU:CD1	1:Q:339:GLN:HB2	2.49	0.42
1:Q:330:GLN:O	1:Q:333:LEU:HD22	2.19	0.42
1:P:335:LEU:HD23	1:Q:101:HIS:NE2	2.34	0.42
1:P:290:SER:O	1:P:295:ARG:NH2	2.53	0.42
1:P:321:LEU:HD23	1:Q:101:HIS:HD2	1.84	0.42
1:Q:128:LEU:HD21	2:Q:6082:HOH:O	2.19	0.42
1:R:339:GLN:CB	1:S:332:LEU:HD11	2.50	0.42
1:P:98:HIS:HA	1:Q:333:LEU:CD1	2.50	0.42
1:S:209:GLU:CB	1:S:212:SER:HB2	2.49	0.42
1:Q:330:GLN:O	1:Q:333:LEU:CD2	2.68	0.42
1:S:76:MET:HE1	1:S:163:HIS:O	2.19	0.42
1:P:99:LEU:H	1:Q:333:LEU:CD2	2.32	0.42
1:P:331:ALA:HA	1:Q:99:LEU:HD22	2.02	0.42
1:S:319:LEU:CD2	1:S:335:LEU:HD22	2.50	0.42
1:R:150:ARG:HH12	1:R:154:LEU:HD12	1.85	0.42
1:R:288:LEU:HD22	1:R:294:PHE:CG	2.54	0.42
1:P:257:GLU:HG3	2:P:6024:HOH:O	2.19	0.41
1:S:140:ILE:HD11	1:S:150:ARG:HB2	2.02	0.41
1:P:56:LYS:O	1:P:57:VAL:HG23	2.20	0.41
1:P:273:ALA:HB3	1:P:276:ILE:HG22	2.01	0.41
1:Q:335:LEU:O	1:Q:336:VAL:HG23	2.20	0.41
1:R:231:VAL:HG11	1:R:278:TYR:HB3	2.02	0.41
1:S:69:LYS:HB2	1:S:170:LEU:O	2.19	0.41
1:P:212:SER:N	1:P:213:PRO:CD	2.83	0.41
1:R:326:ALA:HA	1:R:327:PRO:HD3	1.67	0.41
1:P:231:VAL:CG1	1:P:278:TYR:HB3	2.51	0.41
1:Q:234:ALA:HB3	1:Q:237:LEU:HG	2.01	0.41
1:S:217:LEU:HD22	1:S:258:LEU:HD11	2.03	0.41
1:Q:233:ARG:HA	1:Q:270:GLY:O	2.20	0.41
1:P:67:ASP:HA	1:P:173:VAL:HG23	2.03	0.41
1:Q:153:LEU:HD11	1:Q:237:LEU:HD21	2.02	0.41
1:P:332:LEU:HD22	1:Q:335:LEU:CD2	2.38	0.41
1:Q:73:LEU:HD12	1:Q:73:LEU:HA	1.93	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:170:LEU:C	1:Q:172:GLY:H	2.29	0.41
1:Q:237:LEU:HD12	1:Q:270:GLY:HA2	2.03	0.41
1:R:67:ASP:OD1	1:R:72:GLU:HB2	2.21	0.41
1:R:343:LEU:HD13	1:S:324:THR:O	2.20	0.41
1:S:110:LEU:O	1:S:114:PHE:HB2	2.20	0.41
1:P:116:LYS:HE3	2:P:5933:HOH:O	2.20	0.41
1:R:333:LEU:CG	1:S:98:HIS:HA	2.51	0.41
1:R:337:PRO:HB2	1:S:199:LEU:HD12	2.03	0.41
1:R:345:ARG:HG2	1:R:345:ARG:NH1	2.36	0.41
1:P:242:LEU:C	1:P:242:LEU:HD23	2.46	0.40
1:R:350:SER:C	1:R:352:ALA:H	2.29	0.40
1:S:65:VAL:HG21	1:S:173:VAL:HG21	2.03	0.40
1:P:108:LEU:HD13	1:Q:108:LEU:HD13	2.04	0.40
1:Q:180:ARG:HG2	1:Q:180:ARG:NH1	2.37	0.40
1:P:289:MET:HE3	1:P:289:MET:O	2.20	0.40
1:S:319:LEU:C	1:S:319:LEU:HD23	2.46	0.40
1:P:189:LEU:HA	1:P:190:PRO:HD3	1.93	0.40
1:R:67:ASP:OD2	1:R:70:ASN:HB2	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	P	291/379 (77%)	275 (94%)	14 (5%)	2 (1%)	18	38
1	Q	300/379 (79%)	279 (93%)	11 (4%)	10 (3%)	3	5
1	R	298/379 (79%)	280 (94%)	12 (4%)	6 (2%)	6	12
1	S	291/379 (77%)	275 (94%)	13 (4%)	3 (1%)	12	28
All	All	1180/1516 (78%)	1109 (94%)	50 (4%)	21 (2%)	6	14

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	R	327	PRO
1	Q	204	GLY
1	R	57	VAL
1	R	336	VAL
1	Q	56	LYS
1	Q	202	GLU
1	Q	336	VAL
1	S	202	GLU
1	P	69	LYS
1	P	82	VAL
1	Q	205	ASP
1	Q	327	PRO
1	R	204	GLY
1	Q	69	LYS
1	Q	328	SER
1	S	82	VAL
1	Q	82	VAL
1	R	208	THR
1	S	204	GLY
1	R	82	VAL
1	Q	259	PRO

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	P	251/327 (77%)	224 (89%)	27 (11%)	6	13
1	Q	259/327 (79%)	235 (91%)	24 (9%)	8	18
1	R	257/327 (79%)	237 (92%)	20 (8%)	11	26
1	S	251/327 (77%)	230 (92%)	21 (8%)	10	23
All	All	1018/1308 (78%)	926 (91%)	92 (9%)	9	20

All (92) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	P	57	VAL

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Mol	Chain	Res	Type
1	P	64	LEU
1	P	70	ASN
1	P	88	LEU
1	P	123	LEU
1	P	135	LEU
1	P	139	PHE
1	P	148	GLN
1	P	154	LEU
1	P	160	LYS
1	P	173	VAL
1	P	183	ASP
1	P	190	PRO
1	P	191	GLN
1	P	192	HIS
1	P	203	GLN
1	P	205	ASP
1	P	211	HIS
1	P	223	ASP
1	P	228	LEU
1	P	281	LEU
1	P	288	LEU
1	P	311	LEU
1	P	321	LEU
1	P	333	LEU
1	P	339	GLN
1	P	346	ARG
1	Q	64	LEU
1	Q	65	VAL
1	Q	68	GLU
1	Q	71	GLN
1	Q	88	LEU
1	Q	110	LEU
1	Q	135	LEU
1	Q	152	GLU
1	Q	155	ARG
1	Q	199	LEU
1	Q	211	HIS
1	Q	214	SER
1	Q	216	ILE
1	Q	223	ASP
1	Q	228	LEU
1	Q	252	GLU

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Mol	Chain	Res	Type
1	Q	253	LEU
1	Q	281	LEU
1	Q	288	LEU
1	Q	311	LEU
1	Q	321	LEU
1	Q	329	GLU
1	Q	333	LEU
1	Q	356	SER
1	R	65	VAL
1	R	71	GLN
1	R	88	LEU
1	R	110	LEU
1	R	113	VAL
1	R	123	LEU
1	R	135	LEU
1	R	152	GLU
1	R	154	LEU
1	R	167	LEU
1	R	178	LEU
1	R	212	SER
1	R	228	LEU
1	R	281	LEU
1	R	288	LEU
1	R	311	LEU
1	R	316	ASP
1	R	328	SER
1	R	333	LEU
1	R	341	GLU
1	S	64	LEU
1	S	88	LEU
1	S	113	VAL
1	S	123	LEU
1	S	135	LEU
1	S	148	GLN
1	S	152	GLU
1	S	154	LEU
1	S	167	LEU
1	S	168	GLU
1	S	173	VAL
1	S	199	LEU
1	S	211	HIS
1	S	228	LEU

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Mol	Chain	Res	Type
1	S	252	GLU
1	S	288	LEU
1	S	311	LEU
1	S	321	LEU
1	S	339	GLN
1	S	343	LEU
1	S	348	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	P	71	GLN
1	P	98	HIS
1	P	101	HIS
1	P	144	GLN
1	P	148	GLN
1	P	163	HIS
1	P	191	GLN
1	P	239	GLN
1	P	330	GLN
1	P	339	GLN
1	Q	55	HIS
1	Q	70	ASN
1	Q	87	ASN
1	Q	98	HIS
1	Q	134	GLN
1	Q	163	HIS
1	Q	186	GLN
1	Q	192	HIS
1	Q	203	GLN
1	R	71	GLN
1	R	98	HIS
1	R	134	GLN
1	R	144	GLN
1	R	163	HIS
1	R	203	GLN
1	R	348	GLN
1	S	87	ASN
1	S	98	HIS
1	S	101	HIS
1	S	163	HIS
1	S	191	GLN

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Mol	Chain	Res	Type
1	S	239	GLN
1	S	248	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.