



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 04:16 PM UTC

PDB ID : 4S0S / pdb_00004s0s
Title : STRUCTURE OF HUMAN PREGNANE X RECEPTOR LIGAND BINDING DOMAIN with ADNECTIN-1
Authors : Khan, J.A.
Deposited on : 2015-01-05
Resolution : 2.80 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) : 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

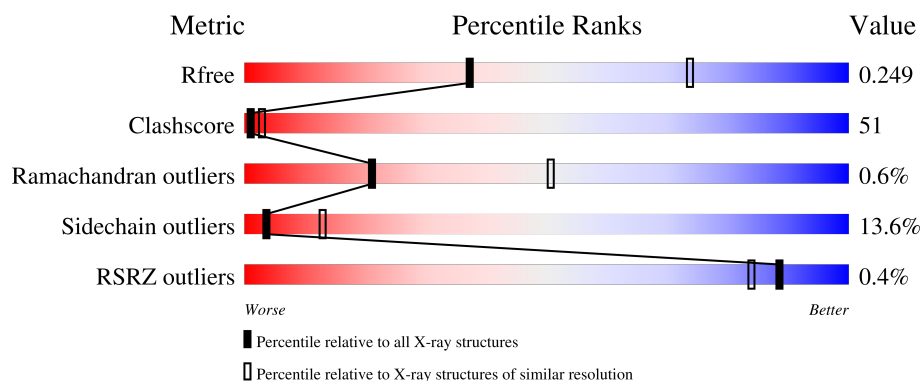
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	315	41% 36% 9% • 13%
1	B	315	43% 37% 5% • 13%
2	D	120	26% 33% 9% 7% 25%
2	E	120	2% 18% 40% 14% • 25%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5622 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 Nuclear receptor subfamily 1 group I member 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	273	Total	C	N	O	S	0	0	0
			2130	1371	354	388	17			
1	B	273	Total	C	N	O	S	0	1	0
			2123	1371	350	384	18			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	120	MET	-	expression tag	UNP O75469
A	121	LYS	-	expression tag	UNP O75469
A	122	LYS	-	expression tag	UNP O75469
A	123	HIS	-	expression tag	UNP O75469
A	124	HIS	-	expression tag	UNP O75469
A	125	HIS	-	expression tag	UNP O75469
A	126	HIS	-	expression tag	UNP O75469
A	127	HIS	-	expression tag	UNP O75469
A	128	HIS	-	expression tag	UNP O75469
A	129	GLY	-	expression tag	UNP O75469
B	120	MET	-	expression tag	UNP O75469
B	121	LYS	-	expression tag	UNP O75469
B	122	LYS	-	expression tag	UNP O75469
B	123	HIS	-	expression tag	UNP O75469
B	124	HIS	-	expression tag	UNP O75469
B	125	HIS	-	expression tag	UNP O75469
B	126	HIS	-	expression tag	UNP O75469
B	127	HIS	-	expression tag	UNP O75469
B	128	HIS	-	expression tag	UNP O75469
B	129	GLY	-	expression tag	UNP O75469

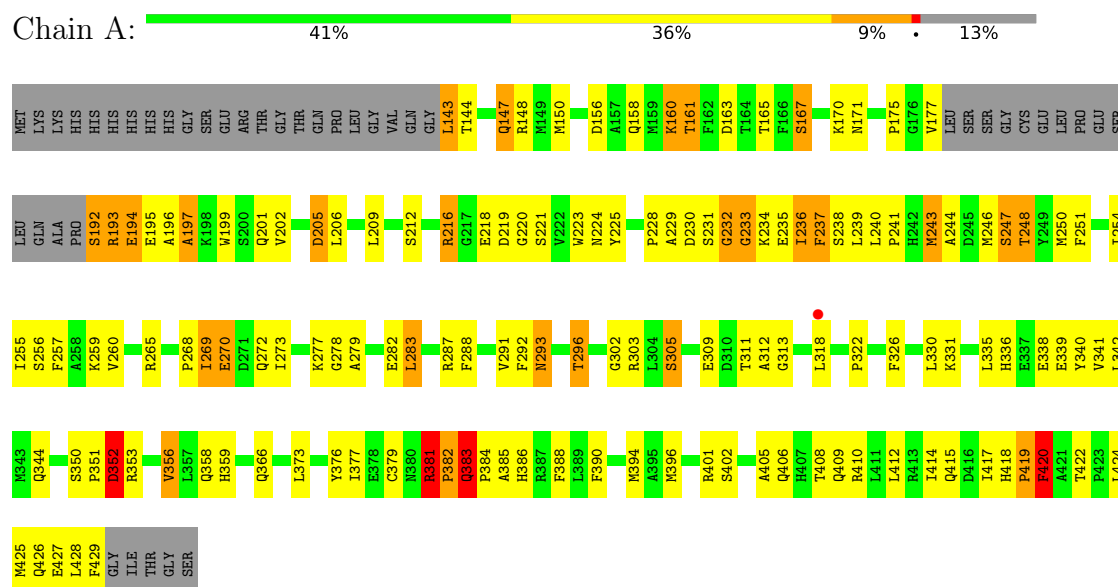
- Molecule 2 is a protein called Adnectin-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	90	Total 684	C 448	N 98	O 136	S 2	0	0	0
2	E	90	Total 685	C 448	N 98	O 137	S 2	0	0	0

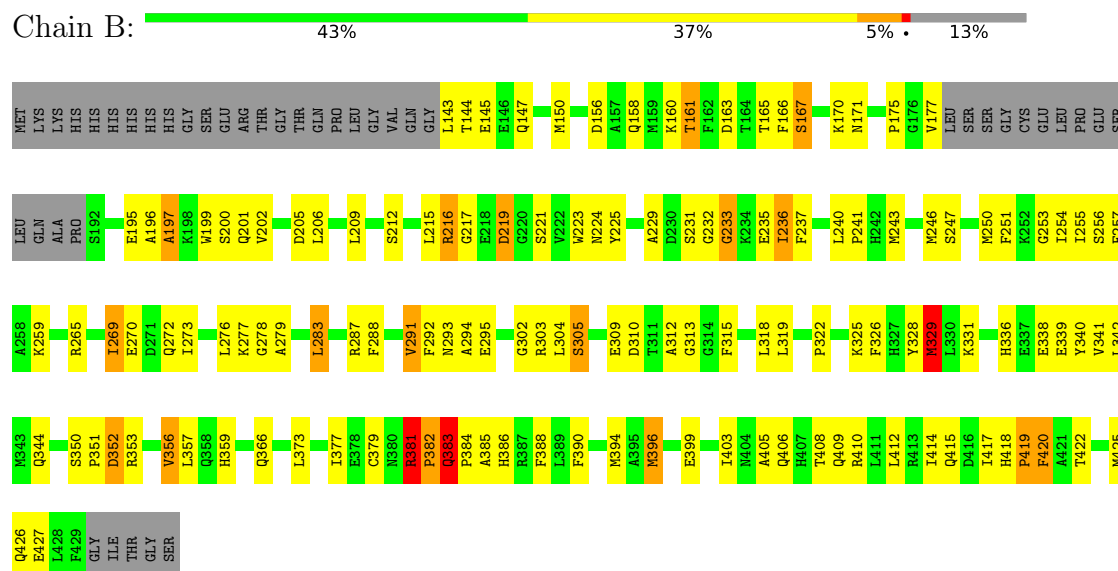
3 Residue-property plots

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.

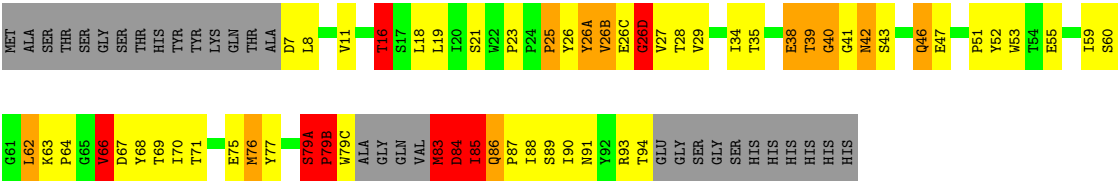
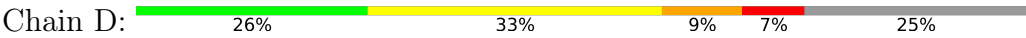
- Molecule 1: Nuclear receptor subfamily 1 group I member 2



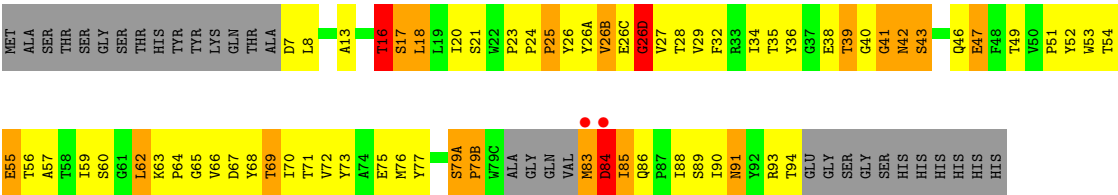
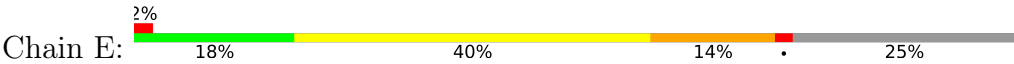
- Molecule 1: Nuclear receptor subfamily 1 group I member 2



● Molecule 2: Adnectin-1



● Molecule 2: Adnectin-1



4 Data and refinement statistics

Property	Value	Source
Space group	P 4	Depositor
Cell constants a, b, c, α , β , γ	119.23Å 119.23Å 83.71Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.91 – 2.80 34.91 – 2.80	Depositor EDS
% Data completeness (in resolution range)	100.0 (34.91-2.80) 99.9 (34.91-2.80)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.35 (at 2.81Å)	Xtriage
Refinement program	BUSTER-TNT BUSTER 2.11.6, BUSTER	Depositor
R, R_{free}	0.216 , 0.229 0.248 , 0.249	Depositor DCC
R_{free} test set	1479 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	85.9	Xtriage
Anisotropy	0.331	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 80.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.488 for h,-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	5622	wwPDB-VP
Average B, all atoms (Å ²)	92.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.00% 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

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	0.49	0/2180	0.70	0/2953
1	B	0.59	2/2176 (0.1%)	2.09	7/2948 (0.2%)
2	D	0.71	1/706 (0.1%)	1.24	3/978 (0.3%)
2	E	0.39	0/707	0.69	0/979
All	All	0.55	3/5769 (0.1%)	1.44	10/7858 (0.1%)

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	18
1	B	0	12
2	D	0	16
2	E	0	12
All	All	0	58

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	66	VAL	C-N	15.92	1.54	1.33
1	B	329[A]	MET	CA-C	10.90	1.67	1.52
1	B	329[B]	MET	CA-C	10.90	1.67	1.52

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	329[A]	MET	CA-C-O	-72.76	16.46	120.51
1	B	329[B]	MET	CA-C-O	-72.76	16.46	120.51
2	D	66	VAL	O-C-N	24.69	148.85	123.18
1	B	328	TYR	CA-C-N	19.99	159.72	121.54
1	B	328	TYR	C-N-CA	19.99	159.72	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	66	VAL	CA-C-N	-14.50	100.28	120.87
2	D	66	VAL	C-N-CA	-14.50	100.28	120.87
1	B	329[A]	MET	CB-CA-C	5.26	120.88	110.42
1	B	329[B]	MET	CB-CA-C	5.26	120.88	110.42
1	B	145	GLU	N-CA-C	-5.24	105.56	111.28

There are no chirality outliers.

All (58) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	192	SER	Peptide
1	A	193	ARG	Peptide
1	A	194	GLU	Peptide
1	A	195	GLU	Peptide
1	A	197	ALA	Peptide
1	A	209	LEU	Peptide
1	A	229	ALA	Peptide
1	A	232	GLY	Peptide
1	A	233	GLY	Peptide
1	A	237	PHE	Peptide
1	A	279	ALA	Peptide
1	A	352	ASP	Peptide
1	A	381	ARG	Peptide
1	A	382	PRO	Peptide
1	A	383	GLN	Peptide
1	A	385	ALA	Peptide
1	A	388	PHE	Peptide
1	A	420	PHE	Peptide
1	B	195	GLU	Peptide
1	B	197	ALA	Peptide
1	B	209	LEU	Peptide
1	B	229	ALA	Peptide
1	B	233	GLY	Peptide
1	B	279	ALA	Peptide
1	B	352	ASP	Peptide
1	B	381	ARG	Peptide
1	B	382	PRO	Peptide
1	B	383	GLN	Peptide
1	B	385	ALA	Peptide
1	B	388	PHE	Peptide
2	D	16	THR	Peptide
2	D	25	PRO	Peptide

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Mol	Chain	Res	Type	Group
2	D	26(A)	TYR	Peptide
2	D	26(B)	VAL	Peptide
2	D	26(D)	GLY	Peptide
2	D	38	GLU	Peptide
2	D	39	THR	Peptide
2	D	40	GLY	Peptide
2	D	41	GLY	Peptide
2	D	66	VAL	Mainchain
2	D	79(A)	SER	Peptide
2	D	79(B)	PRO	Peptide
2	D	83	MET	Peptide
2	D	84	ASP	Peptide
2	D	85	ILE	Peptide
2	D	86	GLN	Peptide
2	E	13	ALA	Peptide
2	E	16	THR	Peptide
2	E	25	PRO	Peptide
2	E	26(B)	VAL	Peptide
2	E	26(D)	GLY	Peptide
2	E	41	GLY	Peptide
2	E	42	ASN	Peptide
2	E	43	SER	Peptide
2	E	79(A)	SER	Peptide
2	E	79(B)	PRO	Peptide
2	E	83	MET	Peptide
2	E	84	ASP	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2130	0	2018	193	0
1	B	2123	0	1998	172	0
2	D	684	0	639	118	0
2	E	685	0	640	103	0
All	All	5622	0	5295	562	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 51.

All (562) 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:352:ASP:CB	1:A:401:ARG:HH22	1.10	1.50
1:A:161:THR:HG21	1:A:257:PHE:CB	1.53	1.38
1:B:161:THR:HG21	1:B:257:PHE:CB	1.54	1.37
1:A:161:THR:HG21	1:A:257:PHE:CA	1.58	1.32
1:A:192:SER:N	1:A:193:ARG:O	1.59	1.32
2:D:63:LYS:O	2:D:94:THR:CG2	1.78	1.30
1:A:233:GLY:HA3	1:A:235:GLU:OE1	1.17	1.30
1:A:231:SER:HB3	1:A:235:GLU:OE2	1.27	1.30
1:B:161:THR:HG21	1:B:257:PHE:CA	1.59	1.30
2:E:26(B):VAL:HG12	2:E:27:VAL:CG1	1.63	1.27
1:B:415:GLN:HA	1:B:418:HIS:O	1.35	1.26
1:A:415:GLN:HA	1:A:418:HIS:O	1.36	1.23
2:D:63:LYS:O	2:D:94:THR:HG21	1.31	1.22
1:B:231:SER:HB3	1:B:235:GLU:OE2	1.09	1.22
2:D:42:ASN:OD1	2:E:42:ASN:CB	1.89	1.20
1:A:382:PRO:O	1:A:384:PRO:HD2	1.39	1.20
1:B:288:PHE:O	1:B:291:VAL:HG23	1.41	1.20
2:D:35:THR:OG1	2:D:71:THR:OG1	1.55	1.19
1:A:219:ASP:OD2	1:A:221:SER:OG	1.61	1.19
1:A:231:SER:CB	1:A:235:GLU:OE2	1.93	1.17
1:B:382:PRO:O	1:B:384:PRO:HD2	1.38	1.17
1:B:231:SER:CB	1:B:235:GLU:OE2	1.95	1.15
2:D:42:ASN:OD1	2:E:42:ASN:HB3	1.01	1.15
1:A:356:VAL:O	1:A:359:HIS:CE1	2.00	1.14
2:D:83:MET:N	2:D:83:MET:SD	2.19	1.14
1:B:156:ASP:OD2	1:B:160:LYS:HE3	1.45	1.13
2:D:42:ASN:CG	2:E:42:ASN:HB3	1.72	1.13
1:B:415:GLN:CA	1:B:418:HIS:O	1.97	1.12
1:A:202:VAL:HG21	1:A:417:ILE:HD13	1.20	1.12
2:E:38:GLU:HB3	2:E:43:SER:OG	1.49	1.11
1:A:415:GLN:CA	1:A:418:HIS:O	1.97	1.11
1:A:219:ASP:OD1	1:A:221:SER:N	1.82	1.10
1:A:353:ARG:O	1:A:356:VAL:HG23	1.49	1.10
2:D:26(D):GLY:HA3	2:D:76:MET:HE3	1.20	1.10
1:A:219:ASP:CG	1:A:221:SER:OG	1.93	1.10
1:B:288:PHE:O	1:B:291:VAL:CG2	1.97	1.10
1:A:161:THR:CG2	1:A:257:PHE:CA	2.29	1.09
1:A:233:GLY:HA3	1:A:235:GLU:CD	1.76	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:161:THR:HG21	1:B:257:PHE:HB2	1.12	1.08
2:D:85:ILE:CG1	2:D:86:GLN:HA	1.82	1.08
1:A:339:GLU:OE1	1:A:381:ARG:NH1	1.87	1.06
1:B:303:ARG:HD3	1:B:303:ARG:H	1.14	1.06
1:B:161:THR:CG2	1:B:257:PHE:CA	2.32	1.06
1:A:161:THR:HG21	1:A:257:PHE:HB2	1.12	1.04
1:B:382:PRO:HD2	1:B:386:HIS:CD2	1.92	1.04
2:D:8:LEU:HD12	2:D:21:SER:O	1.57	1.03
2:D:85:ILE:HG12	2:D:86:GLN:CA	1.89	1.03
1:B:353:ARG:O	1:B:356:VAL:HG23	1.57	1.02
2:D:64:PRO:HA	2:D:94:THR:HB	1.38	1.02
2:E:26(B):VAL:CG1	2:E:27:VAL:HG12	1.89	1.02
1:A:161:THR:HB	1:A:287:ARG:HH22	1.22	1.02
2:D:85:ILE:HG12	2:D:86:GLN:HA	1.05	1.02
1:A:161:THR:CG2	1:A:257:PHE:HB2	1.88	1.02
1:B:161:THR:HB	1:B:287:ARG:HH22	1.23	1.01
1:A:288:PHE:O	1:A:291:VAL:CG2	2.08	1.01
1:A:356:VAL:O	1:A:359:HIS:HE1	1.38	1.01
1:A:293:ASN:CG	1:A:296:THR:OG1	2.04	1.00
1:A:233:GLY:N	1:A:235:GLU:OE2	1.94	1.00
1:B:161:THR:CG2	1:B:257:PHE:HB2	1.90	1.00
1:B:202:VAL:HG21	1:B:417:ILE:HD13	1.42	1.00
2:E:79(A):SER:HB3	2:E:79(B):PRO:HA	1.41	0.99
1:A:303:ARG:H	1:A:303:ARG:HD3	1.19	0.99
1:B:410:ARG:O	1:B:414:ILE:HG13	1.63	0.99
1:A:161:THR:HG21	1:A:257:PHE:HA	1.42	0.98
1:A:233:GLY:CA	1:A:235:GLU:OE1	2.11	0.98
1:A:161:THR:CG2	1:A:257:PHE:HA	1.93	0.98
2:D:42:ASN:HB2	2:E:42:ASN:OD1	1.63	0.98
1:A:288:PHE:O	1:A:291:VAL:HG23	1.62	0.98
2:D:79(A):SER:HB3	2:D:79(B):PRO:HA	1.44	0.97
1:B:161:THR:HG21	1:B:257:PHE:HA	1.46	0.97
1:A:233:GLY:CA	1:A:235:GLU:CD	2.37	0.97
1:A:219:ASP:CG	1:A:221:SER:HG	1.71	0.97
1:A:233:GLY:H	1:A:235:GLU:CD	1.73	0.96
2:E:59:ILE:HG22	2:E:62:LEU:HD21	1.43	0.96
1:A:202:VAL:HG21	1:A:417:ILE:CD1	1.95	0.96
1:A:202:VAL:HG11	1:A:417:ILE:HD11	1.48	0.95
1:B:143:LEU:CD1	1:B:379:CYS:SG	2.54	0.95
2:D:26(C):GLU:N	2:D:26(C):GLU:OE1	1.99	0.95
1:A:352:ASP:HB2	1:A:401:ARG:NH2	1.17	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:25:PRO:CG	2:D:26(A):TYR:HE1	1.80	0.94
1:A:219:ASP:OD1	1:A:221:SER:OG	1.86	0.94
1:B:382:PRO:O	1:B:384:PRO:CD	2.16	0.94
1:B:382:PRO:HD2	1:B:386:HIS:HD2	1.29	0.93
2:D:26(C):GLU:O	2:D:27:VAL:N	2.00	0.93
2:E:25:PRO:HB3	2:E:26:TYR:HB3	1.50	0.93
1:A:353:ARG:HG2	1:A:353:ARG:HH11	1.34	0.93
2:E:26(B):VAL:CG1	2:E:27:VAL:CG1	2.45	0.92
1:B:339:GLU:OE1	1:B:381:ARG:NH1	2.03	0.92
2:E:26(B):VAL:HG12	2:E:27:VAL:HG12	0.94	0.92
1:A:233:GLY:N	1:A:235:GLU:CD	2.28	0.92
1:B:415:GLN:C	1:B:418:HIS:O	2.13	0.92
2:D:64:PRO:HA	2:D:94:THR:CB	2.00	0.91
1:B:161:THR:CG2	1:B:257:PHE:HA	1.99	0.91
2:D:63:LYS:C	2:D:94:THR:HG21	1.95	0.91
1:A:415:GLN:C	1:A:418:HIS:O	2.14	0.90
2:D:26(B):VAL:HA	2:D:26(C):GLU:C	1.96	0.90
2:D:64:PRO:C	2:D:94:THR:HG21	1.96	0.89
1:A:410:ARG:O	1:A:414:ILE:HG13	1.72	0.89
2:D:26(D):GLY:CA	2:D:76:MET:HE3	2.01	0.89
1:A:194:GLU:HA	1:A:196:ALA:H	1.36	0.89
1:A:283:LEU:HD13	1:A:344:GLN:HB3	1.55	0.89
2:D:42:ASN:CB	2:E:42:ASN:OD1	2.21	0.88
2:E:26(B):VAL:HA	2:E:26(C):GLU:C	1.97	0.88
1:B:351:PRO:HD2	1:B:366:GLN:NE2	1.89	0.88
1:B:156:ASP:OD2	1:B:160:LYS:CE	2.21	0.88
2:D:64:PRO:CA	2:D:94:THR:HG21	2.04	0.88
1:A:382:PRO:O	1:A:384:PRO:CD	2.22	0.87
1:B:143:LEU:HD11	1:B:379:CYS:SG	2.12	0.87
1:A:382:PRO:HD2	1:A:386:HIS:CD2	2.10	0.87
2:D:63:LYS:O	2:D:94:THR:HG22	1.71	0.86
1:A:422:THR:OG1	1:A:425:MET:HG3	1.75	0.86
2:D:25:PRO:HB3	2:D:26(A):TYR:CD1	2.10	0.86
2:E:85:ILE:HB	2:E:86:GLN:CB	2.05	0.86
1:A:427:GLU:HG2	2:D:51:PRO:HD2	1.58	0.86
2:E:68:TYR:O	2:E:91:ASN:HB3	1.74	0.85
1:B:322:PRO:HG2	1:B:406:GLN:HE22	1.39	0.85
2:D:25:PRO:CG	2:D:26(A):TYR:CE1	2.60	0.85
2:E:25:PRO:HB3	2:E:26(A):TYR:CD1	2.12	0.84
2:E:26(C):GLU:O	2:E:27:VAL:N	2.09	0.84
1:B:202:VAL:HG11	1:B:417:ILE:HD11	1.57	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:59:ILE:HG22	2:D:62:LEU:HD21	1.60	0.82
1:B:427:GLU:HG2	2:E:51:PRO:HD2	1.61	0.82
2:D:25:PRO:HB3	2:D:26:TYR:HB3	1.58	0.82
1:A:216:ARG:HH11	1:A:216:ARG:HG3	1.45	0.82
1:A:144:THR:OG1	1:A:147:GLN:CG	2.28	0.82
1:B:353:ARG:HG2	1:B:353:ARG:HH11	1.44	0.82
2:D:26(B):VAL:CG2	2:D:26(C):GLU:HA	2.10	0.81
1:A:293:ASN:CB	1:A:296:THR:OG1	2.28	0.81
1:B:161:THR:CG2	1:B:257:PHE:N	2.43	0.81
1:A:322:PRO:HG2	1:A:406:GLN:HE22	1.45	0.81
2:E:35:THR:HA	2:E:46:GLN:O	1.81	0.81
1:A:293:ASN:HB3	1:A:296:THR:OG1	1.80	0.81
1:B:283:LEU:HD13	1:B:344:GLN:HB3	1.63	0.81
1:B:325:LYS:O	1:B:329[B]:MET:HB2	1.81	0.81
1:A:144:THR:OG1	1:A:147:GLN:HG3	1.80	0.80
1:B:144:THR:OG1	1:B:147:GLN:HG3	1.79	0.80
1:A:161:THR:CG2	1:A:257:PHE:CB	2.46	0.80
1:B:356:VAL:O	1:B:359:HIS:NE2	2.14	0.80
1:A:382:PRO:HD2	1:A:386:HIS:HD2	1.44	0.80
2:D:26(B):VAL:HG23	2:D:26(C):GLU:HA	1.63	0.80
1:A:311:THR:OG1	1:A:313:GLY:HA3	1.82	0.79
1:B:351:PRO:CD	1:B:366:GLN:NE2	2.44	0.79
1:A:161:THR:CG2	1:A:257:PHE:N	2.45	0.79
2:D:64:PRO:C	2:D:94:THR:CG2	2.55	0.79
1:B:415:GLN:O	1:B:418:HIS:O	1.98	0.79
1:A:339:GLU:CD	1:A:381:ARG:NH1	2.42	0.78
2:D:25:PRO:CB	2:D:26(A):TYR:CD1	2.67	0.77
1:A:194:GLU:HA	1:A:196:ALA:N	2.00	0.77
1:B:303:ARG:HD3	1:B:303:ARG:N	1.97	0.77
1:A:288:PHE:O	1:A:291:VAL:HG22	1.82	0.77
1:B:161:THR:CG2	1:B:257:PHE:CB	2.48	0.77
1:A:216:ARG:HG3	1:A:216:ARG:NH1	2.00	0.77
2:E:25:PRO:CB	2:E:26:TYR:HB3	2.14	0.77
2:E:39:THR:HG23	2:E:69:THR:OG1	1.84	0.77
1:B:288:PHE:O	1:B:291:VAL:HG22	1.85	0.77
1:A:415:GLN:O	1:A:418:HIS:O	2.02	0.76
1:B:415:GLN:OE1	1:B:419:PRO:HA	1.84	0.76
1:B:158:GLN:HE22	1:B:344:GLN:HE22	1.30	0.76
1:A:283:LEU:CD1	1:A:344:GLN:HB3	2.16	0.76
2:D:64:PRO:CA	2:D:94:THR:CB	2.63	0.76
2:D:71:THR:HG22	2:D:89:SER:OG	1.86	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:422:THR:OG1	1:B:425:MET:HG3	1.85	0.76
2:D:34:ILE:O	2:D:47:GLU:HA	1.86	0.75
2:D:64:PRO:CA	2:D:94:THR:CG2	2.63	0.75
1:A:353:ARG:O	1:A:356:VAL:CG2	2.31	0.75
2:D:25:PRO:HG2	2:D:26(A):TYR:HE1	1.51	0.75
2:D:66:VAL:H	2:D:94:THR:HG23	1.50	0.75
1:B:351:PRO:HD2	1:B:366:GLN:HE22	1.49	0.75
1:B:415:GLN:O	1:B:418:HIS:C	2.30	0.75
1:A:231:SER:HB3	1:A:235:GLU:CD	2.11	0.75
1:B:312:ALA:N	1:B:313:GLY:HA3	2.02	0.75
1:A:312:ALA:N	1:A:313:GLY:HA3	2.02	0.74
1:B:144:THR:HG23	1:B:147:GLN:OE1	1.87	0.74
1:B:273:ILE:O	1:B:277:LYS:HG3	1.86	0.74
1:B:325:LYS:O	1:B:329[A]:MET:HB2	1.87	0.74
2:D:64:PRO:HA	2:D:94:THR:CG2	2.17	0.74
1:A:352:ASP:CB	1:A:401:ARG:NH2	1.92	0.74
1:B:357:LEU:O	1:B:359:HIS:HD2	1.70	0.74
2:D:26(D):GLY:HA3	2:D:76:MET:CE	2.12	0.74
2:D:79(A):SER:HB3	2:D:79(B):PRO:CA	2.17	0.73
2:D:62:LEU:HD23	2:D:62:LEU:N	2.02	0.73
2:E:25:PRO:HB3	2:E:26(A):TYR:H	1.53	0.73
1:A:353:ARG:HG2	1:A:353:ARG:NH1	2.02	0.72
1:B:161:THR:HB	1:B:287:ARG:NH2	2.03	0.72
1:A:244:ALA:O	1:A:248:THR:OG1	2.06	0.72
1:B:143:LEU:HD12	1:B:379:CYS:SG	2.29	0.72
1:A:192:SER:N	1:A:193:ARG:C	2.45	0.72
1:B:283:LEU:CD1	1:B:344:GLN:HB3	2.20	0.72
1:A:351:PRO:HD2	1:A:366:GLN:NE2	2.05	0.72
1:A:246:MET:HE2	1:A:250:MET:HG2	1.71	0.71
1:A:383:GLN:HA	1:A:383:GLN:OE1	1.88	0.71
2:E:34:ILE:O	2:E:47:GLU:HA	1.90	0.71
1:B:196:ALA:O	1:B:197:ALA:HB3	1.90	0.71
2:D:39:THR:HA	2:D:69:THR:OG1	1.89	0.71
1:B:202:VAL:HG21	1:B:417:ILE:CD1	2.19	0.70
2:E:25:PRO:HG3	2:E:26(A):TYR:CZ	2.26	0.70
2:E:65:GLY:N	2:E:94:THR:OG1	2.23	0.70
1:A:415:GLN:O	1:A:418:HIS:C	2.35	0.70
1:A:206:LEU:CD1	1:A:236:ILE:HB	2.21	0.70
2:D:16:THR:O	2:D:62:LEU:HG	1.91	0.70
1:A:219:ASP:CG	1:A:221:SER:H	1.97	0.70
2:D:25:PRO:CB	2:D:26:TYR:HB3	2.20	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:64:PRO:CA	2:D:94:THR:HB	2.15	0.70
1:B:158:GLN:HE22	1:B:344:GLN:NE2	1.90	0.70
1:A:303:ARG:HD3	1:A:303:ARG:N	2.01	0.69
1:B:216:ARG:NH1	1:B:305:SER:OG	2.26	0.69
2:D:35:THR:HA	2:D:46:GLN:O	1.93	0.69
1:B:269:ILE:N	1:B:269:ILE:HD13	2.07	0.69
2:E:25:PRO:HG3	2:E:26(A):TYR:CE1	2.28	0.69
2:E:79(A):SER:HB3	2:E:79(B):PRO:CA	2.20	0.68
2:D:25:PRO:O	2:D:26(B):VAL:HG12	1.93	0.68
2:E:66:VAL:O	2:E:93:ARG:O	2.10	0.68
1:B:156:ASP:O	1:B:160:LYS:HG3	1.93	0.68
1:A:231:SER:OG	1:A:232:GLY:N	2.25	0.68
1:A:293:ASN:C	1:A:293:ASN:HD22	2.02	0.68
1:A:326:PHE:CE2	1:A:396:MET:HG3	2.29	0.68
1:A:292:PHE:O	1:A:331:LYS:HE2	1.94	0.68
1:A:303:ARG:H	1:A:303:ARG:CD	2.01	0.68
2:E:8:LEU:HD12	2:E:21:SER:O	1.93	0.67
1:B:144:THR:OG1	1:B:147:GLN:CG	2.43	0.67
1:A:259:LYS:NZ	2:D:26(C):GLU:HB3	2.09	0.67
2:E:59:ILE:CG2	2:E:62:LEU:HD21	2.20	0.67
1:B:144:THR:N	1:B:147:GLN:OE1	2.20	0.66
1:B:310:ASP:OD1	1:B:312:ALA:HB2	1.95	0.66
1:B:339:GLU:CD	1:B:381:ARG:NH1	2.53	0.66
1:A:352:ASP:HB2	1:A:401:ARG:HH22	0.53	0.66
1:B:163:ASP:OD1	1:B:165:THR:OG1	2.13	0.66
2:E:26(B):VAL:CG1	2:E:27:VAL:HG11	2.25	0.66
1:A:144:THR:OG1	1:A:147:GLN:HG2	1.95	0.66
1:B:310:ASP:CG	1:B:312:ALA:HB2	2.21	0.66
1:B:233:GLY:HA2	1:B:235:GLU:H	1.61	0.66
2:D:25:PRO:CA	2:D:26:TYR:HB3	2.25	0.66
2:E:25:PRO:CA	2:E:26:TYR:HB3	2.26	0.66
1:A:161:THR:HG23	1:A:257:PHE:HA	1.75	0.66
2:D:25:PRO:HG3	2:D:26(A):TYR:HE1	1.59	0.66
1:B:383:GLN:HA	1:B:383:GLN:OE1	1.94	0.66
1:A:143:LEU:O	1:A:148:ARG:NH1	2.29	0.66
2:E:68:TYR:O	2:E:91:ASN:CB	2.42	0.66
1:A:231:SER:OG	1:A:235:GLU:OE2	2.13	0.65
1:A:196:ALA:O	1:A:197:ALA:HB3	1.95	0.65
1:B:382:PRO:C	1:B:384:PRO:CD	2.69	0.65
2:D:26(B):VAL:HG23	2:D:26(C):GLU:CA	2.26	0.65
1:B:197:ALA:HA	1:B:200:SER:H	1.62	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:62:LEU:N	2:E:62:LEU:HD23	2.12	0.65
1:B:293:ASN:C	1:B:293:ASN:HD22	2.03	0.65
1:A:161:THR:HB	1:A:287:ARG:NH2	2.03	0.64
1:A:206:LEU:HD12	1:A:236:ILE:HB	1.79	0.64
1:A:293:ASN:ND2	1:A:296:THR:H	1.96	0.64
2:E:26(B):VAL:CA	2:E:26(C):GLU:C	2.71	0.63
1:B:377:ILE:O	1:B:381:ARG:HB2	1.99	0.63
1:A:223:TRP:CE2	1:B:225:TYR:HD2	2.17	0.63
2:D:25:PRO:CB	2:D:26(A):TYR:HD1	2.11	0.63
2:D:26(B):VAL:CA	2:D:26(C):GLU:C	2.70	0.63
2:D:66:VAL:H	2:D:94:THR:CG2	2.11	0.63
2:E:25:PRO:CG	2:E:26(A):TYR:CZ	2.82	0.62
2:D:66:VAL:O	2:D:93:ARG:HA	1.99	0.62
1:B:336:HIS:N	1:B:339:GLU:OE2	2.27	0.62
2:D:11:VAL:HB	2:D:19:LEU:HD23	1.82	0.62
1:A:382:PRO:C	1:A:384:PRO:CD	2.72	0.62
2:E:26:TYR:CG	2:E:26(A):TYR:HD1	2.18	0.62
1:A:377:ILE:O	1:A:381:ARG:HB2	2.00	0.62
1:A:382:PRO:C	1:A:384:PRO:HD2	2.22	0.61
2:D:25:PRO:CB	2:D:26(A):TYR:CE1	2.82	0.61
1:A:293:ASN:CG	1:A:296:THR:HG1	2.06	0.61
1:A:156:ASP:O	1:A:160:LYS:HG3	1.99	0.61
1:B:353:ARG:O	1:B:356:VAL:CG2	2.40	0.61
2:E:84:ASP:OD1	2:E:84:ASP:N	2.28	0.61
1:A:201:GLN:HA	1:A:201:GLN:NE2	2.15	0.61
2:D:26(B):VAL:CG2	2:D:26(C):GLU:CA	2.78	0.60
1:A:163:ASP:OD1	1:A:165:THR:OG1	2.19	0.60
1:B:353:ARG:HH11	1:B:353:ARG:CG	2.14	0.60
1:B:216:ARG:CG	1:B:216:ARG:HH11	2.14	0.60
2:D:26(B):VAL:HG23	2:D:26(C):GLU:O	2.02	0.60
1:A:216:ARG:HH11	1:A:216:ARG:CG	2.13	0.60
1:B:206:LEU:CD1	1:B:236:ILE:HB	2.32	0.60
2:D:84:ASP:OD2	2:D:85:ILE:HB	2.02	0.60
1:B:351:PRO:CD	1:B:366:GLN:HE22	2.13	0.60
1:B:161:THR:HG23	1:B:257:PHE:HA	1.81	0.59
1:B:309:GLU:HA	1:B:309:GLU:OE1	2.02	0.59
1:A:171:ASN:N	1:A:171:ASN:HD22	2.00	0.59
1:B:143:LEU:HD12	1:B:143:LEU:N	2.18	0.59
1:A:414:ILE:O	1:A:418:HIS:O	2.20	0.59
2:E:93:ARG:O	2:E:94:THR:HG23	2.02	0.58
2:D:27:VAL:HG23	2:D:75:GLU:H	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:293:ASN:HD22	1:B:294:ALA:N	2.01	0.58
2:E:27:VAL:HG23	2:E:75:GLU:O	2.03	0.58
1:A:373:LEU:O	1:A:377:ILE:HG13	2.04	0.58
2:E:26(A):TYR:HD2	2:E:76:MET:HE1	1.69	0.58
2:E:68:TYR:O	2:E:91:ASN:HA	2.02	0.58
1:B:206:LEU:HD12	1:B:236:ILE:HB	1.86	0.58
2:D:26(C):GLU:H	2:D:26(C):GLU:CD	1.98	0.58
1:A:312:ALA:N	1:A:313:GLY:CA	2.67	0.57
1:A:422:THR:O	1:A:426:GLN:HG3	2.03	0.57
1:B:165:THR:HG1	1:B:167:SER:HG	1.47	0.57
2:D:26(B):VAL:HG22	2:D:26(C):GLU:HA	1.84	0.57
1:A:165:THR:O	1:A:302:GLY:HA3	2.04	0.57
1:B:312:ALA:N	1:B:313:GLY:CA	2.67	0.57
2:E:25:PRO:CG	2:E:26(A):TYR:CE1	2.87	0.57
2:D:25:PRO:HB3	2:D:26(A):TYR:CE1	2.39	0.57
2:E:25:PRO:HB3	2:E:26(A):TYR:CE1	2.38	0.57
1:B:292:PHE:O	1:B:331:LYS:HE2	2.05	0.57
2:D:42:ASN:CB	2:E:42:ASN:CG	2.78	0.57
1:A:225:TYR:HD2	1:B:223:TRP:CE2	2.23	0.56
1:A:336:HIS:N	1:A:339:GLU:OE2	2.33	0.56
1:A:259:LYS:HZ2	2:D:26(C):GLU:HB3	1.71	0.56
1:B:175:PRO:HB2	1:B:225:TYR:CE2	2.41	0.56
1:B:420:PHE:CD1	1:B:420:PHE:N	2.73	0.56
1:A:233:GLY:CA	1:A:235:GLU:OE2	2.50	0.56
1:B:196:ALA:O	1:B:197:ALA:CB	2.54	0.56
2:D:26(A):TYR:CD1	2:D:26(A):TYR:N	2.73	0.56
2:D:39:THR:CA	2:D:69:THR:OG1	2.54	0.56
2:E:25:PRO:O	2:E:26(B):VAL:HG22	2.05	0.56
1:B:177:VAL:HG12	1:B:177:VAL:O	2.06	0.55
1:B:240:LEU:N	1:B:241:PRO:CD	2.68	0.55
2:D:26(B):VAL:HA	2:D:26(D):GLY:N	2.20	0.55
2:D:7:ASP:O	2:D:23:PRO:HD3	2.06	0.55
1:A:196:ALA:O	1:A:197:ALA:CB	2.53	0.55
1:A:272:GLN:NE2	2:D:52:TYR:OH	2.39	0.55
1:B:303:ARG:H	1:B:303:ARG:CD	1.97	0.55
1:A:383:GLN:N	1:A:384:PRO:CD	2.69	0.55
1:B:415:GLN:CD	1:B:419:PRO:HA	2.31	0.55
1:B:293:ASN:ND2	1:B:295:GLU:H	2.05	0.55
2:E:26(A):TYR:CD1	2:E:26(A):TYR:N	2.73	0.55
2:E:26(B):VAL:HA	2:E:26(D):GLY:N	2.22	0.55
1:B:338:GLU:O	1:B:341:VAL:HG12	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:25:PRO:HG2	2:D:26(A):TYR:CE1	2.32	0.55
1:A:206:LEU:HD13	1:A:236:ILE:HB	1.88	0.55
1:A:240:LEU:N	1:A:241:PRO:CD	2.70	0.55
1:A:338:GLU:O	1:A:341:VAL:HG12	2.07	0.54
2:E:91:ASN:N	2:E:91:ASN:OD1	2.40	0.54
1:A:237:PHE:O	1:A:240:LEU:HB2	2.06	0.54
1:B:422:THR:O	1:B:426:GLN:HG3	2.07	0.54
2:D:42:ASN:CG	2:E:42:ASN:CB	2.62	0.54
1:A:351:PRO:HD2	1:A:366:GLN:HE22	1.70	0.54
2:D:25:PRO:HA	2:D:26:TYR:HB3	1.88	0.54
2:D:26(A):TYR:HB2	2:D:79(C):TRP:HA	1.89	0.54
1:B:383:GLN:N	1:B:384:PRO:CD	2.71	0.54
2:D:68:TYR:O	2:D:91:ASN:HA	2.06	0.54
1:A:420:PHE:CD1	1:A:420:PHE:N	2.73	0.54
2:E:24:PRO:HD3	2:E:55:GLU:OE1	2.08	0.54
1:A:230:ASP:O	1:A:235:GLU:CG	2.55	0.54
1:A:206:LEU:HD12	1:A:236:ILE:HD12	1.89	0.53
1:B:225:TYR:CD1	1:B:225:TYR:C	2.86	0.53
1:B:250:MET:O	1:B:254:ILE:HG12	2.08	0.53
2:D:77:TYR:CD1	2:D:77:TYR:C	2.85	0.53
2:D:25:PRO:HA	2:D:26:TYR:CB	2.38	0.53
2:D:85:ILE:HG13	2:D:87:PRO:HD3	1.91	0.53
1:A:427:GLU:HG2	2:D:51:PRO:CD	2.35	0.53
2:E:41:GLY:O	2:E:42:ASN:HB2	2.07	0.53
1:B:339:GLU:OE2	1:B:381:ARG:NH1	2.42	0.53
2:E:77:TYR:CD1	2:E:77:TYR:C	2.85	0.53
2:E:16:THR:O	2:E:62:LEU:HG	2.09	0.53
2:E:25:PRO:HA	2:E:26:TYR:CB	2.38	0.53
1:B:357:LEU:O	1:B:359:HIS:CD2	2.58	0.52
1:B:359:HIS:CD2	1:B:359:HIS:H	2.26	0.52
2:E:25:PRO:HA	2:E:26:TYR:HB3	1.91	0.52
1:B:251:PHE:O	1:B:255:ILE:HG13	2.09	0.52
2:D:26(B):VAL:HG23	2:D:26(C):GLU:C	2.34	0.52
2:E:25:PRO:CA	2:E:26:TYR:CB	2.86	0.52
2:E:68:TYR:O	2:E:91:ASN:CA	2.57	0.52
1:A:143:LEU:HD11	1:A:376:TYR:HA	1.92	0.52
1:A:230:ASP:O	1:A:235:GLU:OE2	2.28	0.52
1:B:143:LEU:CD1	1:B:143:LEU:N	2.73	0.52
2:E:71:THR:HG22	2:E:89:SER:OG	2.10	0.52
1:A:230:ASP:OD1	1:A:231:SER:O	2.27	0.52
1:B:353:ARG:CG	1:B:353:ARG:NH1	2.73	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:25:PRO:HG3	2:D:26(A):TYR:CE1	2.39	0.52
2:D:25:PRO:CA	2:D:26:TYR:CB	2.88	0.52
2:D:27:VAL:HG23	2:D:75:GLU:O	2.09	0.52
1:A:260:VAL:O	1:A:265:ARG:NH1	2.41	0.51
2:D:42:ASN:HB3	2:E:42:ASN:OD1	2.09	0.51
1:B:383:GLN:O	1:B:386:HIS:N	2.33	0.51
1:A:205:ASP:HB3	1:A:410:ARG:HD3	1.92	0.51
1:B:373:LEU:O	1:B:377:ILE:HG13	2.09	0.51
1:B:215:LEU:CD1	1:B:304:LEU:HD23	2.41	0.51
2:E:93:ARG:C	2:E:94:THR:HG23	2.35	0.51
1:A:228:PRO:HB3	1:B:219:ASP:HB2	1.92	0.51
1:B:216:ARG:NH1	1:B:216:ARG:CG	2.73	0.51
2:E:26:TYR:CD1	2:E:26(A):TYR:N	2.79	0.51
1:A:352:ASP:OD1	1:A:352:ASP:N	2.44	0.51
1:A:415:GLN:OE1	1:A:419:PRO:HA	2.11	0.51
1:B:216:ARG:HH11	1:B:216:ARG:HG2	1.75	0.51
1:B:278:GLY:HA3	1:B:353:ARG:HD3	1.91	0.51
2:D:26:TYR:CD1	2:D:26(A):TYR:N	2.79	0.51
1:A:282:GLU:OE2	1:A:353:ARG:NH2	2.40	0.51
1:B:382:PRO:CD	1:B:386:HIS:HD2	2.14	0.51
2:E:16:THR:O	2:E:62:LEU:HB2	2.11	0.51
1:A:339:GLU:OE2	1:A:381:ARG:NH1	2.38	0.50
1:B:326:PHE:CE1	1:B:396:MET:HG3	2.46	0.50
1:B:399:GLU:O	1:B:403:ILE:HG13	2.11	0.50
1:A:250:MET:O	1:A:254:ILE:HG12	2.12	0.50
1:A:251:PHE:O	1:A:255:ILE:HG13	2.12	0.50
1:B:427:GLU:HG2	2:E:51:PRO:CD	2.38	0.50
1:A:216:ARG:NH2	1:A:305:SER:OG	2.37	0.50
1:B:414:ILE:O	1:B:418:HIS:O	2.29	0.50
2:D:68:TYR:O	2:D:91:ASN:HB3	2.12	0.50
1:A:352:ASP:HB2	1:A:401:ARG:HH21	1.52	0.50
2:E:51:PRO:HB2	2:E:53:TRP:CE2	2.47	0.50
1:B:269:ILE:O	1:B:273:ILE:HG13	2.12	0.49
1:A:147:GLN:HA	1:A:150:MET:HE3	1.94	0.49
1:A:177:VAL:HG12	1:A:177:VAL:O	2.10	0.49
1:A:219:ASP:OD1	1:A:220:GLY:N	2.45	0.49
1:B:359:HIS:CD2	1:B:359:HIS:N	2.80	0.49
1:A:158:GLN:HE22	1:A:344:GLN:NE2	2.09	0.49
2:E:17:SER:O	2:E:18:LEU:HD12	2.11	0.49
1:A:273:ILE:HG22	1:A:277:LYS:HD2	1.95	0.49
2:E:42:ASN:N	2:E:42:ASN:HD22	2.10	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:201:GLN:OE1	1:B:201:GLN:HA	2.11	0.49
1:A:230:ASP:O	1:A:235:GLU:HG3	2.12	0.49
2:D:27:VAL:HA	2:D:75:GLU:O	2.12	0.49
1:B:310:ASP:OD2	1:B:312:ALA:HB2	2.13	0.48
1:B:158:GLN:OE1	1:B:287:ARG:NH2	2.36	0.48
1:B:165:THR:O	1:B:302:GLY:HA3	2.12	0.48
1:A:243:MET:O	1:A:247:SER:OG	2.31	0.48
1:A:175:PRO:HB2	1:A:225:TYR:CE2	2.49	0.48
2:E:7:ASP:O	2:E:23:PRO:HD3	2.13	0.48
1:A:256:SER:OG	2:D:28:THR:HG21	2.12	0.48
1:A:415:GLN:CD	1:A:419:PRO:HA	2.39	0.48
2:D:64:PRO:N	2:D:94:THR:HG21	2.25	0.48
2:E:26:TYR:CD1	2:E:26:TYR:C	2.91	0.48
2:E:34:ILE:HD12	2:E:34:ILE:N	2.28	0.48
2:E:38:GLU:O	2:E:40:GLY:O	2.32	0.48
1:A:201:GLN:HA	1:A:201:GLN:HE21	1.78	0.47
1:B:408:THR:O	1:B:412:LEU:HG	2.14	0.47
2:E:36:TYR:CE2	2:E:59:ILE:HG23	2.49	0.47
1:A:278:GLY:HA3	1:A:353:ARG:HD3	1.96	0.47
2:E:35:THR:HG22	2:E:47:GLU:HB3	1.96	0.47
2:E:70:ILE:O	2:E:89:SER:HA	2.14	0.47
1:A:158:GLN:HE22	1:A:344:GLN:HE22	1.60	0.47
2:D:42:ASN:HB3	2:E:42:ASN:CG	2.39	0.47
1:B:197:ALA:H	1:B:199:TRP:H	1.62	0.47
2:E:73:TYR:CD1	2:E:73:TYR:N	2.82	0.47
1:A:170:LYS:O	1:A:171:ASN:HB2	2.15	0.46
1:A:205:ASP:N	1:A:205:ASP:OD1	2.48	0.46
1:B:197:ALA:N	1:B:199:TRP:H	2.12	0.46
1:B:293:ASN:HD21	1:B:295:GLU:HG3	1.80	0.46
2:E:16:THR:O	2:E:62:LEU:CB	2.63	0.46
1:A:144:THR:CB	1:A:147:GLN:HG3	2.45	0.46
2:D:46:GLN:HE21	2:D:46:GLN:HB2	1.57	0.46
2:D:67:ASP:OD1	2:D:68:TYR:N	2.49	0.46
2:E:29:VAL:HG11	2:E:49:THR:HB	1.97	0.46
1:B:396:MET:HE3	1:B:396:MET:HA	1.97	0.46
1:A:293:ASN:C	1:A:293:ASN:ND2	2.73	0.46
2:E:34:ILE:HG13	2:E:72:VAL:HG22	1.97	0.46
1:A:165:THR:HG1	1:A:167:SER:HG	1.53	0.46
1:A:239:LEU:HD23	1:A:239:LEU:HA	1.81	0.46
2:D:7:ASP:O	2:D:23:PRO:CD	2.64	0.46
2:E:25:PRO:CB	2:E:26(A):TYR:H	2.25	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:89:SER:O	2:E:90:ILE:CG2	2.64	0.46
1:A:353:ARG:NH1	1:A:353:ARG:CG	2.73	0.45
1:B:383:GLN:N	1:B:384:PRO:HD3	2.31	0.45
1:A:408:THR:O	1:A:412:LEU:HG	2.15	0.45
1:B:205:ASP:HB3	1:B:410:ARG:HD3	1.99	0.45
2:D:27:VAL:O	2:D:52:TYR:HB3	2.16	0.45
2:E:20:ILE:CG1	2:E:57:ALA:HB3	2.46	0.45
2:E:85:ILE:HB	2:E:86:GLN:CA	2.46	0.45
1:B:233:GLY:HA2	1:B:235:GLU:N	2.30	0.45
1:B:170:LYS:O	1:B:171:ASN:HB2	2.16	0.45
1:A:330:LEU:HD12	1:A:330:LEU:O	2.17	0.45
1:A:351:PRO:CD	1:A:366:GLN:NE2	2.76	0.45
1:B:256:SER:OG	2:E:28:THR:HG21	2.17	0.45
2:D:26:TYR:CD1	2:D:26:TYR:C	2.94	0.45
1:B:340:TYR:O	1:B:344:GLN:HG3	2.16	0.44
2:D:39:THR:O	2:D:69:THR:OG1	2.32	0.44
2:D:39:THR:HG23	2:D:40:GLY:H	1.81	0.44
1:A:428:LEU:O	1:A:429:PHE:CD1	2.70	0.44
1:B:143:LEU:HD11	1:B:379:CYS:CB	2.47	0.44
1:B:215:LEU:HD11	1:B:304:LEU:CD2	2.48	0.44
2:E:26:TYR:C	2:E:26:TYR:HD1	2.26	0.44
2:E:54:THR:HG22	2:E:56:THR:H	1.83	0.44
1:A:390:PHE:O	1:A:394:MET:HG2	2.18	0.44
1:B:273:ILE:HG22	1:B:277:LYS:HE3	2.00	0.44
1:A:350:SER:HB2	1:A:353:ARG:HG3	1.98	0.43
1:B:254:ILE:HD12	1:B:283:LEU:HB3	1.99	0.43
1:A:216:ARG:HH22	1:A:305:SER:HG	1.62	0.43
1:A:144:THR:N	1:A:147:GLN:HG3	2.33	0.43
1:A:309:GLU:OE1	1:A:309:GLU:HA	2.18	0.43
1:B:246:MET:HE2	1:B:250:MET:HG2	2.00	0.43
1:B:293:ASN:C	1:B:293:ASN:ND2	2.73	0.43
2:D:66:VAL:HG12	2:D:67:ASP:O	2.18	0.43
1:A:219:ASP:OD1	1:A:221:SER:CB	2.65	0.43
1:B:233:GLY:N	1:B:235:GLU:OE2	2.33	0.43
1:B:390:PHE:O	1:B:394:MET:HG2	2.17	0.43
1:B:405:ALA:O	1:B:409:GLN:HG2	2.18	0.43
1:B:165:THR:O	1:B:166:PHE:HB2	2.18	0.43
1:A:144:THR:H	1:A:147:GLN:HG3	1.83	0.43
1:A:335:LEU:HA	1:A:339:GLU:OE2	2.17	0.43
2:E:63:LYS:HA	2:E:64:PRO:HD3	1.84	0.43
1:B:161:THR:HG22	1:B:253:GLY:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:342:LEU:HD13	1:B:373:LEU:HA	2.01	0.43
1:B:259:LYS:O	1:B:265:ARG:NH1	2.49	0.43
1:B:288:PHE:C	1:B:291:VAL:CG2	2.85	0.43
2:E:85:ILE:CB	2:E:86:GLN:CA	2.97	0.43
1:B:233:GLY:CA	1:B:235:GLU:H	2.31	0.43
1:A:259:LYS:HZ1	2:D:26(C):GLU:HB3	1.82	0.43
1:B:310:ASP:OD1	1:B:312:ALA:N	2.52	0.42
1:B:359:HIS:HD2	1:B:359:HIS:H	1.67	0.42
1:B:420:PHE:H	1:B:420:PHE:HD1	1.60	0.42
1:A:342:LEU:HD13	1:A:373:LEU:HA	2.01	0.42
1:B:167:SER:O	1:B:170:LYS:HE3	2.19	0.42
1:A:405:ALA:O	1:A:409:GLN:HG2	2.19	0.42
1:A:268:PRO:HG2	1:A:358:GLN:HG3	2.02	0.42
1:A:402:SER:O	1:A:406:GLN:HG3	2.20	0.42
1:A:424:LEU:HD12	2:D:51:PRO:HD3	2.01	0.42
1:B:288:PHE:C	1:B:291:VAL:HG22	2.42	0.42
2:E:25:PRO:CB	2:E:26(A):TYR:CE1	3.02	0.42
1:A:219:ASP:CG	1:A:221:SER:CB	2.91	0.42
1:B:235:GLU:H	1:B:235:GLU:CD	2.25	0.42
1:B:276:LEU:HD23	1:B:276:LEU:HA	1.93	0.42
2:D:25:PRO:O	2:D:26(B):VAL:CG1	2.63	0.42
1:A:197:ALA:N	1:A:199:TRP:H	2.17	0.42
1:A:420:PHE:H	1:A:420:PHE:HD1	1.61	0.42
1:B:144:THR:CG2	1:B:147:GLN:OE1	2.63	0.42
2:D:25:PRO:HB2	2:D:26(A):TYR:HD1	1.83	0.42
2:D:51:PRO:HB2	2:D:53:TRP:CE2	2.55	0.42
2:E:27:VAL:O	2:E:52:TYR:HB3	2.20	0.42
1:A:269:ILE:HG23	1:A:270:GLU:N	2.35	0.42
1:A:197:ALA:H	1:A:199:TRP:H	1.66	0.42
1:A:340:TYR:O	1:A:344:GLN:HG3	2.19	0.42
2:E:89:SER:O	2:E:90:ILE:HG22	2.19	0.42
1:A:331:LYS:HD2	1:A:331:LYS:HA	1.83	0.42
1:A:167:SER:O	1:A:170:LYS:HE3	2.20	0.41
2:E:26(A):TYR:HD2	2:E:76:MET:CE	2.30	0.41
1:A:422:THR:HG1	1:A:425:MET:HG3	1.80	0.41
2:D:29:VAL:O	2:D:75:GLU:HB2	2.21	0.41
1:A:288:PHE:C	1:A:291:VAL:HG22	2.45	0.41
1:B:206:LEU:HD13	1:B:236:ILE:HB	2.00	0.41
2:E:26(C):GLU:H	2:E:26(C):GLU:HG3	1.62	0.41
1:B:237:PHE:O	1:B:240:LEU:HB2	2.20	0.41
2:D:27:VAL:HG23	2:D:75:GLU:N	2.34	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:39:THR:HB	2:D:68:TYR:CA	2.50	0.41
2:E:85:ILE:H	2:E:85:ILE:HG13	1.60	0.41
1:B:315:PHE:O	1:B:319:LEU:N	2.40	0.41
2:D:85:ILE:HG13	2:D:86:GLN:HA	1.91	0.41
2:E:25:PRO:HB3	2:E:26(A):TYR:N	2.27	0.41
1:A:409:GLN:HA	1:A:409:GLN:NE2	2.36	0.41
1:B:231:SER:OG	1:B:232:GLY:N	2.53	0.41
1:B:272:GLN:NE2	2:E:52:TYR:OH	2.52	0.41
1:B:350:SER:HA	1:B:351:PRO:HD2	1.89	0.41
1:A:202:VAL:CG1	1:A:417:ILE:HD11	2.35	0.41
1:B:331:LYS:HD2	1:B:331:LYS:HA	1.73	0.41
2:D:39:THR:HG23	2:D:40:GLY:N	2.35	0.41
1:B:217:GLY:HA3	1:B:219:ASP:OD1	2.21	0.41
2:D:8:LEU:CD1	2:D:21:SER:O	2.49	0.41
2:E:29:VAL:CG1	2:E:49:THR:HB	2.51	0.41
1:A:238:SER:O	1:A:241:PRO:HD2	2.21	0.41
2:D:70:ILE:O	2:D:89:SER:HA	2.21	0.41
2:E:7:ASP:O	2:E:23:PRO:CD	2.69	0.41
2:E:89:SER:C	2:E:90:ILE:HG23	2.45	0.41
1:A:161:THR:HG22	1:A:257:PHE:N	2.34	0.41
1:A:383:GLN:N	1:A:384:PRO:HD3	2.35	0.41
1:B:147:GLN:HA	1:B:150:MET:HE3	2.02	0.41
1:B:382:PRO:C	1:B:384:PRO:HD3	2.44	0.41
2:D:26(A):TYR:CD1	2:D:26(A):TYR:C	2.98	0.41
2:D:38:GLU:HB3	2:D:43:SER:HB3	2.02	0.40
1:A:143:LEU:HD12	1:A:379:CYS:SG	2.62	0.40
2:E:89:SER:C	2:E:90:ILE:CG2	2.94	0.40
2:D:64:PRO:O	2:D:66:VAL:HG23	2.22	0.40
2:E:41:GLY:O	2:E:42:ASN:CB	2.68	0.40
1:A:233:GLY:O	1:A:234:LYS:CB	2.69	0.40
1:B:240:LEU:HD23	1:B:240:LEU:HA	1.81	0.40
2:E:29:VAL:HG12	2:E:32:PHE:N	2.34	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	A	269/315 (85%)	263 (98%)	5 (2%)	1 (0%)	30	60
1	B	270/315 (86%)	262 (97%)	7 (3%)	1 (0%)	30	60
2	D	86/120 (72%)	83 (96%)	2 (2%)	1 (1%)	10	34
2	E	86/120 (72%)	81 (94%)	4 (5%)	1 (1%)	10	34
All	All	711/870 (82%)	689 (97%)	18 (2%)	4 (1%)	21	51

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	26(D)	GLY
2	E	26(D)	GLY
1	A	419	PRO
1	B	419	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	218/279 (78%)	192 (88%)	26 (12%)	5	17
1	B	214/279 (77%)	190 (89%)	24 (11%)	6	19
2	D	75/102 (74%)	60 (80%)	15 (20%)	1	4
2	E	75/102 (74%)	60 (80%)	15 (20%)	1	4
All	All	582/762 (76%)	502 (86%)	80 (14%)	3	13

All (80) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	143	LEU
1	A	147	GLN

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Mol	Chain	Res	Type
1	A	160	LYS
1	A	161	THR
1	A	167	SER
1	A	205	ASP
1	A	212	SER
1	A	216	ARG
1	A	218	GLU
1	A	224	ASN
1	A	236	ILE
1	A	243	MET
1	A	247	SER
1	A	248	THR
1	A	269	ILE
1	A	270	GLU
1	A	283	LEU
1	A	293	ASN
1	A	296	THR
1	A	305	SER
1	A	318	LEU
1	A	352	ASP
1	A	356	VAL
1	A	381	ARG
1	A	383	GLN
1	A	420	PHE
1	B	161	THR
1	B	167	SER
1	B	212	SER
1	B	216	ARG
1	B	219	ASP
1	B	221	SER
1	B	224	ASN
1	B	236	ILE
1	B	243	MET
1	B	247	SER
1	B	269	ILE
1	B	270	GLU
1	B	283	LEU
1	B	291	VAL
1	B	305	SER
1	B	318	LEU
1	B	329[A]	MET
1	B	329[B]	MET

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Mol	Chain	Res	Type
1	B	352	ASP
1	B	356	VAL
1	B	381	ARG
1	B	383	GLN
1	B	396	MET
1	B	420	PHE
2	D	16	THR
2	D	18	LEU
2	D	42	ASN
2	D	46	GLN
2	D	55	GLU
2	D	60	SER
2	D	62	LEU
2	D	76	MET
2	D	79(A)	SER
2	D	79(B)	PRO
2	D	83	MET
2	D	84	ASP
2	D	85	ILE
2	D	88	ILE
2	D	90	ILE
2	E	16	THR
2	E	17	SER
2	E	18	LEU
2	E	39	THR
2	E	47	GLU
2	E	55	GLU
2	E	60	SER
2	E	62	LEU
2	E	67	ASP
2	E	69	THR
2	E	83	MET
2	E	84	ASP
2	E	85	ILE
2	E	88	ILE
2	E	91	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	168	HIS
1	A	171	ASN

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Mol	Chain	Res	Type
1	A	201	GLN
1	A	224	ASN
1	A	272	GLN
1	A	293	ASN
1	A	344	GLN
1	A	359	HIS
1	A	366	GLN
1	A	386	HIS
1	A	406	GLN
1	A	407	HIS
1	A	409	GLN
1	B	168	HIS
1	B	171	ASN
1	B	272	GLN
1	B	293	ASN
1	B	344	GLN
1	B	359	HIS
1	B	366	GLN
1	B	386	HIS
1	B	406	GLN
1	B	409	GLN
2	D	46	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 [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	273/315 (86%)	-0.82	1 (0%) 88 84	57, 85, 125, 160	0
1	B	273/315 (86%)	-0.80	0 100 100	46, 85, 125, 161	1 (0%)
2	D	90/120 (75%)	-0.53	0 100 100	25, 105, 144, 180	0
2	E	90/120 (75%)	-0.39	2 (2%) 62 52	25, 106, 144, 180	0
All	All	726/870 (83%)	-0.72	3 (0%) 88 84	25, 90, 131, 180	1 (0%)

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	318	LEU	2.5
2	E	83	MET	2.4
2	E	84	ASP	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.