



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 11:38 AM UTC

PDB ID : 3T06 / pdb_00003t06
Title : Crystal Structure of the DH/PH fragment of PDZRHOGF with N-terminal regulatory elements in complex with Human RhoA
Authors : Bielnicki, J.A.; Derewenda, U.; Derewenda, Z.S.
Deposited on : 2011-07-19
Resolution : 2.84 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

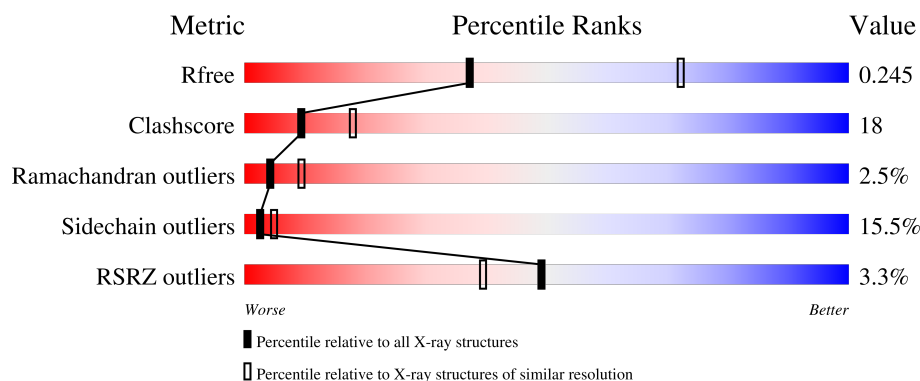
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.84 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	1520 (2.86-2.82)
Clashscore	190562	1559 (2.86-2.82)
Ramachandran outliers	187476	1517 (2.86-2.82)
Sidechain outliers	187428	1518 (2.86-2.82)
RSRZ outliers	180081	1521 (2.86-2.82)

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	418	3% 49% 27% 7% 15%
1	E	418	4% 52% 24% 9% 14%
2	B	178	2% 57% 38% 5%
2	F	178	2% 58% 36% 6%

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 8657 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 Rho guanine nucleotide exchange factor 11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	355	Total	C	N	O	S	0	0	0
			2905	1837	519	534	15			
1	E	358	Total	C	N	O	S	0	0	0
			2930	1852	525	538	15			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1082	HIS	-	expression tag	UNP O15085
A	1083	HIS	-	expression tag	UNP O15085
A	1084	HIS	-	expression tag	UNP O15085
A	1085	HIS	-	expression tag	UNP O15085
A	1086	HIS	-	expression tag	UNP O15085
A	1087	HIS	-	expression tag	UNP O15085
A	1088	HIS	-	expression tag	UNP O15085
A	1089	HIS	-	expression tag	UNP O15085
E	1082	HIS	-	expression tag	UNP O15085
E	1083	HIS	-	expression tag	UNP O15085
E	1084	HIS	-	expression tag	UNP O15085
E	1085	HIS	-	expression tag	UNP O15085
E	1086	HIS	-	expression tag	UNP O15085
E	1087	HIS	-	expression tag	UNP O15085
E	1088	HIS	-	expression tag	UNP O15085
E	1089	HIS	-	expression tag	UNP O15085

- Molecule 2 is a protein called Transforming protein RhoA.

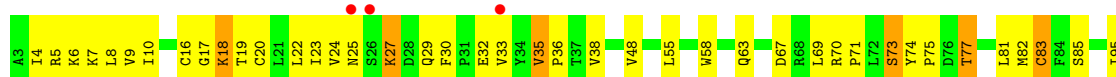
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	178	Total	C	N	O	S	0	0	0
			1411	889	240	272	10			
2	F	178	Total	C	N	O	S	0	0	0
			1411	889	240	272	10			

There are 2 discrepancies between the modelled and reference sequences:

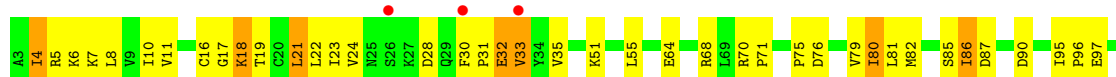
Chain	Residue	Modelled	Actual	Comment	Reference
B	25	ASN	PHE	engineered mutation	UNP P61586
F	25	ASN	PHE	engineered mutation	UNP P61586



• Molecule 2: Transforming protein RhoA



• Molecule 2: Transforming protein RhoA



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	84.37Å 118.63Å 92.44Å 90.00° 113.61° 90.00°	Depositor
Resolution (Å)	29.82 – 2.84 29.82 – 2.84	Depositor EDS
% Data completeness (in resolution range)	93.5 (29.82-2.84) 93.5 (29.82-2.84)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.49 (at 2.85Å)	Xtriage
Refinement program	PHENIX dev_818	Depositor
R, R_{free}	0.208 , 0.257 0.201 , 0.245	Depositor DCC
R_{free} test set	1849 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	58.6	Xtriage
Anisotropy	0.412	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 35.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	8657	wwPDB-VP
Average B, all atoms (Å ²)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.83% 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	0.63	0/2949	1.01	5/3970 (0.1%)
1	E	0.63	0/2975	0.94	5/4004 (0.1%)
2	B	0.60	0/1438	0.99	2/1944 (0.1%)
2	F	0.63	0/1438	1.00	3/1944 (0.2%)
All	All	0.63	0/8800	0.98	15/11862 (0.1%)

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1052	GLY	CA-C-N	13.78	134.58	120.38
1	A	1052	GLY	C-N-CA	13.78	134.58	120.38
1	E	836	GLN	N-CA-C	6.84	118.73	111.28
1	A	838	ILE	CB-CA-C	-6.61	103.39	112.24
2	F	115	VAL	N-CA-C	6.56	117.08	107.37
1	A	1053	PRO	N-CA-C	6.43	118.55	110.70
1	E	1001	GLU	N-CA-C	-5.83	105.48	112.59
2	F	159	CYS	N-CA-C	5.75	115.99	107.88
1	A	748	SER	N-CA-C	-5.57	105.60	112.90
1	E	950	ASN	CA-C-N	5.54	126.76	119.84
1	E	950	ASN	C-N-CA	5.54	126.76	119.84
1	E	1046	ILE	N-CA-C	5.52	114.32	106.53
2	B	170	VAL	N-CA-C	5.38	116.15	110.72
2	B	35	VAL	CB-CA-C	-5.32	106.00	110.94
2	F	79	VAL	N-CA-C	5.24	115.27	108.35

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	A	2905	0	2997	112	0
1	E	2930	0	3022	103	0
2	B	1411	0	1402	58	0
2	F	1411	0	1402	48	0
All	All	8657	0	8823	314	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 18.

All (314) 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:900:THR:HG22	1:A:902:GLU:H	1.33	0.91
1:A:764:MET:HE2	1:A:857:MET:HE1	1.52	0.90
1:E:1056:ILE:HD12	1:E:1056:ILE:H	1.39	0.87
1:A:1053:PRO:HB3	1:A:1054:PRO:HD2	1.58	0.86
2:F:18:LYS:NZ	2:F:64:GLU:OE2	2.10	0.85
2:F:30:PHE:CD1	2:F:31:PRO:HD2	2.13	0.84
1:A:947:ARG:HG3	1:A:948:ALA:H	1.43	0.82
1:E:941:ASP:HB3	1:E:1004:LEU:HB3	1.64	0.80
1:A:1046:ILE:HG23	1:A:1056:ILE:HG13	1.64	0.78
1:A:1034:ARG:HH11	1:A:1035:SER:H	1.28	0.78
1:A:825:LEU:HD23	1:A:916:ILE:HD13	1.67	0.77
1:A:884:LYS:HG3	2:B:38:VAL:HG22	1.70	0.74
2:F:122:ARG:NH2	2:F:158:GLU:OE1	2.22	0.73
2:B:85:SER:OG	2:B:118:LYS:HD2	1.89	0.73
1:A:943:THR:O	1:A:945:LEU:N	2.21	0.73
2:B:16:CYS:HB2	2:B:85:SER:HB2	1.71	0.72
1:A:856:PHE:HD1	1:A:857:MET:HE2	1.55	0.72
1:A:900:THR:HG22	1:A:902:GLU:N	2.05	0.72
2:F:16:CYS:HB2	2:F:85:SER:HB2	1.71	0.71
1:E:976:ILE:HD12	1:E:980:LYS:HE3	1.72	0.71
1:E:950:ASN:ND2	1:E:1021:THR:O	2.24	0.71
1:E:898:GLY:O	1:E:900:THR:HG23	1.91	0.70
2:F:117:ASN:OD1	2:F:118:LYS:N	2.24	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1005:LEU:HD12	1:E:1005:LEU:O	1.91	0.70
1:E:1067:LYS:HE3	1:E:1071:MET:HE2	1.72	0.70
1:A:717:GLN:HG3	1:A:737:GLU:OE2	1.91	0.70
1:E:1026:LEU:HD21	1:E:1057:TYR:CE1	2.27	0.70
2:B:157:MET:HG2	2:B:170:VAL:HG22	1.72	0.69
2:F:21:LEU:HD22	2:F:171:PHE:HE2	1.57	0.69
1:E:1036:VAL:HG22	1:E:1044:PHE:CE2	2.28	0.69
1:E:1056:ILE:HD12	1:E:1056:ILE:N	2.07	0.69
1:E:943:THR:C	1:E:945:LEU:H	2.01	0.68
1:E:1067:LYS:CE	1:E:1071:MET:HE2	2.24	0.68
1:A:816:ARG:O	1:A:816:ARG:HD3	1.91	0.68
1:A:1026:LEU:HD21	1:A:1057:TYR:CE1	2.29	0.67
1:E:816:ARG:O	1:E:816:ARG:HD3	1.94	0.67
2:F:6:LYS:HD2	2:F:178:ALA:HB1	1.76	0.67
2:B:24:VAL:HG12	2:B:30:PHE:HA	1.77	0.67
1:A:879:MET:HE1	2:B:63:GLN:CD	2.19	0.67
1:A:879:MET:HE3	2:B:69:LEU:HB3	1.75	0.67
2:F:19:THR:O	2:F:23:ILE:HG12	1.95	0.67
1:E:926:GLN:OE1	1:E:926:GLN:HA	1.95	0.67
1:A:715:ASN:HD22	1:A:718:HIS:CD2	2.13	0.66
2:F:85:SER:OG	2:F:118:LYS:HD3	1.95	0.66
1:A:826:GLN:HB2	1:A:919:TYR:CD1	2.30	0.66
2:B:100:THR:N	2:B:101:PRO:HD2	2.10	0.66
1:E:941:ASP:HB2	1:E:1002:LYS:HE2	1.78	0.66
1:E:1048:THR:O	1:E:1050:LYS:HG3	1.96	0.66
1:A:945:LEU:HD22	1:A:1005:LEU:HB3	1.78	0.66
2:B:119:LYS:C	2:B:121:LEU:H	2.04	0.65
1:A:738:VAL:HG11	1:A:891:SER:HB3	1.79	0.64
1:A:856:PHE:CD1	1:A:857:MET:HE2	2.32	0.64
1:A:764:MET:HE2	1:A:857:MET:CE	2.27	0.64
1:E:1048:THR:O	1:E:1050:LYS:N	2.30	0.64
1:E:717:GLN:HG2	1:E:737:GLU:OE2	1.98	0.64
1:A:870:GLN:HG3	2:B:5:ARG:HH12	1.62	0.63
1:A:943:THR:C	1:A:945:LEU:H	2.05	0.63
1:E:765:LYS:O	1:E:772:ARG:NH2	2.31	0.63
2:F:4:ILE:O	2:F:4:ILE:HG13	1.98	0.63
2:F:162:LYS:H	2:F:162:LYS:HD2	1.63	0.63
2:F:81:LEU:HD23	2:F:113:ILE:HG12	1.81	0.63
1:E:964:ARG:HD3	1:E:992:LEU:HD12	1.82	0.62
1:A:728:LEU:HD22	1:A:732:GLU:HG2	1.82	0.61
1:E:1064:SER:O	1:E:1068:ASN:OD1	2.18	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1034:ARG:HH11	1:A:1035:SER:N	1.97	0.61
1:A:1053:PRO:HB3	1:A:1054:PRO:CD	2.30	0.61
1:E:978:LYS:O	1:E:979:ASP:HB2	2.00	0.61
2:F:80:ILE:HD13	2:F:103:VAL:HG13	1.82	0.61
2:B:24:VAL:HG23	2:B:25:ASN:H	1.66	0.60
1:E:937:GLN:HA	1:E:937:GLN:OE1	2.01	0.60
2:B:95:ILE:O	2:B:100:THR:HG23	2.02	0.60
1:E:1031:VAL:HG12	1:E:1047:CYS:HA	1.84	0.60
1:A:1040:LYS:H	1:A:1040:LYS:HD3	1.68	0.59
2:F:175:THR:O	2:F:179:LEU:HG	2.02	0.59
2:B:166:GLY:O	2:B:170:VAL:HG23	2.03	0.59
1:A:977:SER:HB2	1:A:980:LYS:HB3	1.83	0.59
1:E:810:SER:HB2	1:E:905:LYS:HB3	1.83	0.59
1:A:1040:LYS:HE2	1:A:1041:ARG:NH1	2.17	0.58
2:B:17:GLY:HA3	2:B:117:ASN:HD22	1.68	0.58
1:A:967:ILE:HD12	1:A:988:LEU:HD13	1.85	0.58
1:A:1026:LEU:HD21	1:A:1057:TYR:CZ	2.38	0.58
1:A:914:ARG:O	1:A:918:LYS:HG3	2.04	0.58
1:E:740:ASN:O	1:E:744:VAL:HG23	2.03	0.58
2:B:19:THR:O	2:B:23:ILE:HG13	2.04	0.58
1:A:1053:PRO:CB	1:A:1054:PRO:HD2	2.31	0.58
1:E:778:LEU:O	1:E:780:PRO:HD3	2.04	0.57
1:E:781:ASN:HD21	1:E:831:GLN:HB3	1.69	0.57
1:E:997:GLN:HB3	1:E:1004:LEU:HD12	1.86	0.57
1:A:729:THR:HG23	1:A:732:GLU:H	1.70	0.57
1:E:1040:LYS:O	1:E:1067:LYS:HD3	2.04	0.57
1:A:764:MET:CE	1:A:857:MET:HE1	2.32	0.57
1:E:1008:HIS:O	1:E:1021:THR:HB	2.04	0.57
2:B:113:ILE:O	2:B:113:ILE:HG13	2.04	0.56
2:B:10:ILE:HD11	2:B:83:CYS:SG	2.45	0.56
1:E:778:LEU:C	1:E:780:PRO:HD3	2.30	0.56
1:E:814:LEU:HD11	1:E:905:LYS:HG2	1.86	0.56
1:E:770:MET:HE1	1:E:843:ILE:HD11	1.86	0.56
2:B:157:MET:HB2	2:B:173:MET:HE1	1.87	0.56
1:A:1053:PRO:CB	1:A:1054:PRO:CD	2.84	0.56
2:F:122:ARG:HH22	2:F:158:GLU:CD	2.14	0.56
1:E:985:HIS:HB2	1:E:998:LYS:HE3	1.86	0.55
2:F:162:LYS:HD2	2:F:162:LYS:N	2.21	0.55
2:B:82:MET:SD	2:B:100:THR:HG22	2.47	0.55
1:E:854:GLN:O	1:E:854:GLN:HG2	2.05	0.55
1:A:1034:ARG:NH1	1:A:1035:SER:H	2.00	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:125:GLU:OE1	2:B:129:ARG:NH1	2.40	0.55
2:B:157:MET:HE3	2:B:157:MET:HA	1.89	0.55
1:A:814:LEU:HD11	1:A:905:LYS:HG2	1.88	0.55
1:E:1065:SER:HA	1:E:1068:ASN:OD1	2.07	0.55
2:B:10:ILE:HG23	2:B:10:ILE:O	2.05	0.55
2:F:140:LYS:HB3	2:F:142:GLU:OE1	2.06	0.55
2:B:122:ARG:NH1	2:B:139:VAL:O	2.37	0.55
1:A:1065:SER:O	1:A:1069:THR:HG23	2.08	0.54
1:E:976:ILE:HD11	1:E:982:LEU:HG	1.88	0.54
1:A:947:ARG:O	1:A:948:ALA:HB3	2.08	0.54
1:E:965:LYS:HG2	1:E:990:GLU:HG3	1.90	0.54
1:A:1036:VAL:HG12	1:A:1037:ALA:N	2.23	0.54
1:E:1049:SER:O	1:E:1050:LYS:O	2.25	0.54
1:A:1034:ARG:NH1	1:A:1035:SER:HB3	2.23	0.54
1:E:876:ILE:HG12	1:E:876:ILE:O	2.07	0.54
2:F:86:ILE:O	2:F:139:VAL:HG23	2.08	0.54
2:B:6:LYS:HD2	2:B:178:ALA:HB1	1.89	0.54
1:E:720:VAL:HG12	1:E:804:PRO:HB3	1.90	0.54
2:F:21:LEU:HD22	2:F:171:PHE:CE2	2.41	0.54
2:B:157:MET:CG	2:B:170:VAL:HG22	2.39	0.54
1:E:759:ILE:HG22	1:E:860:ALA:HB1	1.90	0.54
1:A:941:ASP:HB3	1:A:1004:LEU:HD23	1.90	0.53
1:A:743:PHE:HB3	1:A:800:ARG:HH21	1.73	0.53
2:B:63:GLN:O	2:B:70:ARG:HG3	2.08	0.53
1:A:1046:ILE:HG12	1:A:1056:ILE:HD11	1.89	0.53
1:E:863:HIS:ND1	1:E:864:PRO:HD2	2.23	0.53
1:A:766:LYS:O	1:A:766:LYS:HG3	2.07	0.53
1:E:724:VAL:C	1:E:726:ALA:H	2.16	0.53
1:A:1040:LYS:HE2	1:A:1041:ARG:HH12	1.74	0.52
1:E:959:LEU:HD22	1:E:961:LEU:HD23	1.92	0.52
1:A:975:ARG:HG3	1:A:981:THR:HG22	1.89	0.52
1:E:822:ARG:HD2	1:E:826:GLN:OE1	2.09	0.52
1:E:943:THR:C	1:E:945:LEU:N	2.68	0.52
1:A:728:LEU:HD11	1:A:805:ILE:CD1	2.40	0.52
2:B:24:VAL:HG23	2:B:25:ASN:N	2.25	0.52
1:E:946:GLU:HG2	1:E:957:LYS:HB2	1.91	0.52
2:F:17:GLY:HA3	2:F:117:ASN:ND2	2.25	0.52
2:B:17:GLY:O	2:B:18:LYS:C	2.52	0.51
1:A:950:ASN:ND2	1:A:952:LEU:HB2	2.25	0.51
1:E:933:LEU:HD11	1:E:966:MET:HB2	1.92	0.51
1:A:978:LYS:O	1:A:980:LYS:N	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:122:ARG:HH22	2:B:158:GLU:CD	2.18	0.51
1:E:967:ILE:HD13	1:E:967:ILE:N	2.25	0.51
1:A:863:HIS:HD2	1:A:865:GLN:H	1.57	0.51
2:B:157:MET:HG2	2:B:170:VAL:CG2	2.38	0.51
1:A:1046:ILE:HG23	1:A:1056:ILE:CG1	2.36	0.51
2:F:81:LEU:CD2	2:F:113:ILE:HG12	2.40	0.51
1:A:1036:VAL:HG12	1:A:1037:ALA:H	1.75	0.51
1:A:937:GLN:OE1	1:A:960:ASP:HA	2.11	0.50
1:E:1026:LEU:HD21	1:E:1057:TYR:CD1	2.45	0.50
1:A:1035:SER:HB2	1:A:1071:MET:HE2	1.93	0.50
1:A:945:LEU:HD13	1:A:1005:LEU:O	2.11	0.50
1:A:976:ILE:HG23	1:A:980:LYS:HD3	1.93	0.50
2:B:10:ILE:HG21	2:B:22:LEU:HD11	1.92	0.50
2:F:82:MET:HG2	2:F:95:ILE:HD12	1.94	0.50
1:E:733:ILE:O	1:E:737:GLU:HG2	2.12	0.50
1:E:787:GLU:OE1	1:E:787:GLU:HA	2.12	0.50
2:F:80:ILE:HD13	2:F:103:VAL:CG1	2.42	0.50
1:A:1031:VAL:HA	1:A:1046:ILE:O	2.12	0.49
1:A:739:ILE:HG12	1:A:809:ILE:HD12	1.95	0.49
1:A:968:HIS:HB2	1:A:1073:LEU:HD13	1.94	0.49
1:E:937:GLN:NE2	1:E:960:ASP:HA	2.28	0.49
2:B:110:VAL:HG13	2:B:111:PRO:HD2	1.94	0.49
1:A:873:ASP:O	1:A:876:ILE:HG22	2.13	0.49
1:E:863:HIS:CG	1:E:864:PRO:HD2	2.48	0.49
1:E:716:TRP:HB3	1:E:737:GLU:OE1	2.13	0.48
1:A:987:LEU:HB2	1:A:994:VAL:HG22	1.93	0.48
2:B:70:ARG:HG3	2:B:70:ARG:HH11	1.78	0.48
1:E:1040:LYS:HB2	1:E:1064:SER:HB3	1.95	0.48
2:F:22:LEU:HD23	2:F:171:PHE:HZ	1.78	0.48
1:A:984:LEU:HD13	1:A:995:LEU:HD22	1.95	0.48
1:A:759:ILE:HG22	1:A:860:ALA:HB1	1.96	0.48
1:E:1061:ALA:HB1	1:E:1066:ASP:HB3	1.96	0.48
1:E:788:ILE:HG22	1:E:789:HIS:N	2.28	0.48
1:E:879:MET:SD	1:E:879:MET:C	2.96	0.48
1:E:1070:TRP:O	1:E:1074:LEU:HB2	2.13	0.48
2:F:17:GLY:O	2:F:18:LYS:C	2.56	0.48
1:E:999:GLN:HB3	1:E:1002:LYS:HB3	1.94	0.48
1:A:1040:LYS:HD3	1:A:1040:LYS:N	2.29	0.48
2:B:163:THR:O	2:B:164:LYS:HB2	2.14	0.48
1:E:1068:ASN:OD1	1:E:1068:ASN:N	2.36	0.48
1:A:863:HIS:CD2	1:A:864:PRO:HD2	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:978:LYS:HD2	1:E:979:ASP:H	1.78	0.47
1:A:1021:THR:O	1:A:1055:GLN:NE2	2.47	0.47
1:A:1056:ILE:O	1:A:1056:ILE:HG22	2.14	0.47
1:E:722:LYS:O	1:E:725:VAL:HG12	2.14	0.47
1:E:943:THR:O	1:E:945:LEU:N	2.46	0.47
1:E:1035:SER:HG	1:E:1067:LYS:HZ1	1.54	0.47
2:B:81:LEU:HD23	2:B:113:ILE:CG1	2.45	0.47
2:F:68:ARG:HD2	2:F:68:ARG:HA	1.64	0.47
2:B:24:VAL:O	2:B:25:ASN:C	2.55	0.47
1:E:964:ARG:CD	1:E:992:LEU:HD12	2.45	0.47
2:F:157:MET:HE3	2:F:158:GLU:H	1.80	0.47
1:A:974:TRP:CZ2	1:A:1057:TYR:CD2	3.03	0.47
1:A:1034:ARG:HH12	1:A:1035:SER:HB3	1.80	0.47
1:E:918:LYS:HB3	1:E:918:LYS:HE2	1.66	0.47
1:A:888:LEU:HD12	1:A:888:LEU:HA	1.73	0.47
1:A:951:PRO:HA	1:A:954:ALA:HB2	1.97	0.46
1:A:976:ILE:CG2	1:A:980:LYS:HD3	2.45	0.46
2:B:23:ILE:HD13	2:B:36:PRO:HD2	1.97	0.46
1:E:717:GLN:CG	1:E:737:GLU:OE2	2.62	0.46
1:A:950:ASN:HD22	1:A:952:LEU:HD13	1.79	0.46
1:E:1010:LYS:HE2	1:E:1010:LYS:C	2.41	0.46
1:A:1070:TRP:O	1:A:1074:LEU:HB2	2.15	0.46
2:B:142:GLU:H	2:B:142:GLU:CD	2.24	0.46
1:E:870:GLN:HG3	2:F:5:ARG:HH12	1.80	0.46
1:E:871:LEU:O	1:E:871:LEU:HD22	2.15	0.46
1:E:729:THR:HG23	1:E:732:GLU:H	1.81	0.46
2:F:120:ASP:OD1	2:F:160:SER:HB2	2.15	0.46
1:A:933:LEU:CD2	1:A:966:MET:HE2	2.45	0.46
2:F:95:ILE:HB	2:F:96:PRO:HD3	1.97	0.46
2:F:100:THR:N	2:F:101:PRO:HD2	2.30	0.46
1:E:952:LEU:H	1:E:952:LEU:HD12	1.81	0.46
1:A:750:LEU:HD23	1:A:750:LEU:HA	1.74	0.46
2:B:48:VAL:HG23	2:B:48:VAL:O	2.15	0.46
2:B:179:LEU:O	2:B:180:GLN:C	2.58	0.46
2:F:110:VAL:HG13	2:F:111:PRO:HD2	1.98	0.45
1:A:876:ILE:HG12	1:A:876:ILE:O	2.16	0.45
2:B:7:LYS:HE3	2:B:58:TRP:CE2	2.51	0.45
2:F:108:PRO:O	2:F:109:ASN:HB2	2.16	0.45
2:B:119:LYS:O	2:B:121:LEU:N	2.48	0.45
1:E:1036:VAL:HG13	1:E:1044:PHE:HE2	1.81	0.45
1:E:724:VAL:C	1:E:726:ALA:N	2.73	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:959:LEU:O	1:A:960:ASP:HB2	2.17	0.45
1:A:1040:LYS:H	1:A:1040:LYS:CD	2.24	0.45
1:E:960:ASP:OD1	1:E:963:THR:HG23	2.17	0.45
1:E:781:ASN:ND2	1:E:831:GLN:HB3	2.30	0.45
1:E:879:MET:O	1:E:883:THR:HG23	2.17	0.45
1:A:770:MET:HB2	1:A:771:PRO:HD2	1.99	0.45
2:B:9:VAL:HG22	2:B:58:TRP:HB2	1.99	0.45
1:A:734:ASP:O	1:A:738:VAL:HG23	2.17	0.45
1:A:937:GLN:O	1:A:937:GLN:HG3	2.17	0.45
2:B:117:ASN:CG	2:B:118:LYS:H	2.25	0.45
1:E:1048:THR:C	1:E:1050:LYS:H	2.25	0.45
1:A:971:PRO:O	1:A:972:LEU:HD13	2.17	0.44
1:E:1031:VAL:O	1:E:1032:LEU:HD13	2.17	0.44
2:B:74:TYR:N	2:B:75:PRO:CD	2.80	0.44
2:B:119:LYS:C	2:B:121:LEU:N	2.71	0.44
1:E:1046:ILE:HG13	1:E:1056:ILE:HG23	1.98	0.44
1:A:1032:LEU:HD23	1:A:1032:LEU:HA	1.85	0.44
1:E:1075:GLU:O	1:E:1078:VAL:HG12	2.16	0.44
2:F:10:ILE:HG23	2:F:10:ILE:O	2.16	0.44
2:F:87:ASP:OD1	2:F:87:ASP:C	2.60	0.44
2:F:166:GLY:O	2:F:170:VAL:HG23	2.17	0.44
1:A:999:GLN:HG2	1:A:1004:LEU:CD1	2.48	0.44
2:F:157:MET:HB3	2:F:170:VAL:HG22	1.99	0.44
1:A:1005:LEU:HD23	1:A:1005:LEU:HA	1.82	0.44
1:E:715:ASN:OD1	2:F:33:VAL:HG11	2.17	0.44
1:A:977:SER:HB2	1:A:980:LYS:HD2	1.99	0.44
1:A:751:ARG:HH22	1:A:867:ARG:HD3	1.83	0.44
1:A:943:THR:HG22	1:A:944:ALA:N	2.32	0.44
2:B:100:THR:N	2:B:101:PRO:CD	2.80	0.44
1:A:890:GLU:OE1	1:A:914:ARG:NH2	2.50	0.44
2:F:75:PRO:O	2:F:76:ASP:HB2	2.17	0.43
2:B:103:VAL:O	2:B:107:CYS:HB2	2.17	0.43
2:F:122:ARG:NH1	2:F:139:VAL:O	2.40	0.43
2:F:154:PHE:CD2	2:F:177:ALA:HB2	2.52	0.43
1:E:974:TRP:CD1	1:E:974:TRP:C	2.95	0.43
1:E:1065:SER:HB3	2:F:97:GLU:HG3	1.99	0.43
2:B:77:THR:HG22	2:B:110:VAL:HG11	1.99	0.43
1:A:737:GLU:HA	1:A:737:GLU:OE1	2.18	0.43
2:B:70:ARG:N	2:B:71:PRO:CD	2.81	0.43
2:F:110:VAL:CG1	2:F:111:PRO:HD2	2.48	0.43
1:A:799:LEU:C	1:A:801:GLU:N	2.75	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:816:ARG:HD3	1:E:816:ARG:C	2.42	0.43
2:F:157:MET:CB	2:F:170:VAL:HG22	2.48	0.43
1:E:724:VAL:O	1:E:726:ALA:N	2.52	0.43
1:E:978:LYS:HD2	1:E:979:ASP:N	2.32	0.43
1:E:1067:LYS:HE2	1:E:1071:MET:HE2	1.98	0.42
1:A:782:LEU:HB3	1:A:783:PRO:HD3	1.99	0.42
1:A:816:ARG:HD3	1:A:816:ARG:C	2.41	0.42
1:E:743:PHE:O	1:E:746:GLU:HB3	2.20	0.42
1:A:946:GLU:CB	1:A:957:LYS:HD2	2.50	0.42
2:B:17:GLY:HA3	2:B:117:ASN:ND2	2.31	0.42
2:F:70:ARG:N	2:F:71:PRO:CD	2.81	0.42
2:B:69:LEU:O	2:B:70:ARG:C	2.63	0.42
1:A:1035:SER:HB2	1:A:1071:MET:CE	2.49	0.42
2:B:70:ARG:O	2:B:73:SER:HB2	2.20	0.42
2:F:95:ILE:HB	2:F:96:PRO:CD	2.50	0.42
1:E:1046:ILE:O	1:E:1046:ILE:HG22	2.20	0.42
2:F:21:LEU:CD2	2:F:167:VAL:HG13	2.50	0.42
1:E:775:LEU:HD12	1:E:775:LEU:HA	1.84	0.42
1:A:787:GLU:OE1	1:A:787:GLU:HA	2.20	0.42
1:A:807:LYS:HE2	1:A:807:LYS:HB2	1.87	0.42
1:E:781:ASN:OD1	1:E:781:ASN:N	2.49	0.42
1:E:986:VAL:HG22	1:E:1070:TRP:CH2	2.55	0.42
1:A:900:THR:HG21	1:A:902:GLU:HB3	2.02	0.41
1:A:1073:LEU:HD23	1:A:1073:LEU:HA	1.78	0.41
1:E:992:LEU:HD22	1:E:1025:VAL:CG1	2.50	0.41
1:A:735:ARG:HD2	1:A:895:HIS:O	2.20	0.41
2:F:24:VAL:HG12	2:F:30:PHE:HA	2.02	0.41
2:B:174:ALA:O	2:B:177:ALA:HB3	2.20	0.41
1:E:1048:THR:C	1:E:1050:LYS:N	2.78	0.41
1:A:728:LEU:HD11	1:A:805:ILE:HD13	2.03	0.41
2:B:8:LEU:C	2:B:8:LEU:HD23	2.45	0.41
1:A:977:SER:O	1:A:978:LYS:C	2.63	0.41
1:A:871:LEU:C	1:A:871:LEU:HD22	2.46	0.41
1:A:959:LEU:O	1:A:960:ASP:CB	2.69	0.41
2:B:27:LYS:O	2:B:29:GLN:HG2	2.21	0.41
2:B:129:ARG:O	2:B:132:ALA:HB3	2.20	0.41
1:E:781:ASN:ND2	1:E:831:GLN:OE1	2.54	0.41
1:E:946:GLU:HA	1:E:957:LYS:HB3	2.04	0.40
1:A:933:LEU:HG	1:A:966:MET:HE2	2.03	0.40
1:E:809:ILE:O	1:E:811:ASP:N	2.54	0.40
1:E:873:ASP:OD1	1:E:873:ASP:N	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:889:LEU:HD23	1:A:889:LEU:HA	1.94	0.40
1:A:999:GLN:HG2	1:A:1004:LEU:HD11	2.04	0.40
2:B:95:ILE:HG22	2:B:96:PRO:N	2.37	0.40
1:A:946:GLU:HA	1:A:957:LYS:HD2	2.03	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	351/418 (84%)	310 (88%)	31 (9%)	10 (3%)	4	8
1	E	354/418 (85%)	316 (89%)	28 (8%)	10 (3%)	4	8
2	B	176/178 (99%)	159 (90%)	14 (8%)	3 (2%)	7	15
2	F	176/178 (99%)	158 (90%)	15 (8%)	3 (2%)	7	15
All	All	1057/1192 (89%)	943 (89%)	88 (8%)	26 (2%)	4	9

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	944	ALA
1	A	948	ALA
1	A	959	LEU
1	A	979	ASP
1	A	1053	PRO
2	B	120	ASP
1	E	1049	SER
1	E	1050	LYS
2	B	67	ASP
1	E	944	ALA
1	E	962	THR

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Mol	Chain	Res	Type
1	E	1048	THR
1	A	807	LYS
2	B	18	LYS
1	E	810	SER
1	E	1040	LYS
2	F	18	LYS
1	A	999	GLN
2	F	32	GLU
1	A	720	VAL
1	A	960	ASP
1	E	722	LYS
1	A	800	ARG
1	E	979	ASP
2	F	33	VAL
1	E	725	VAL

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	323/380 (85%)	264 (82%)	59 (18%)	2	2
1	E	326/380 (86%)	273 (84%)	53 (16%)	2	4
2	B	156/156 (100%)	139 (89%)	17 (11%)	6	12
2	F	156/156 (100%)	136 (87%)	20 (13%)	4	8
All	All	961/1072 (90%)	812 (84%)	149 (16%)	2	5

All (149) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	720	VAL
1	A	722	LYS
1	A	729	THR
1	A	731	ARG
1	A	744	VAL
1	A	750	LEU

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Mol	Chain	Res	Type
1	A	755	VAL
1	A	758	LEU
1	A	765	LYS
1	A	766	LYS
1	A	778	LEU
1	A	797	LYS
1	A	805	ILE
1	A	806	ILE
1	A	809	ILE
1	A	812	LEU
1	A	816	ARG
1	A	841	GLU
1	A	842	LEU
1	A	847	GLN
1	A	865	GLN
1	A	871	LEU
1	A	875	ILE
1	A	876	ILE
1	A	882	LEU
1	A	884	LYS
1	A	887	LEU
1	A	888	LEU
1	A	891	SER
1	A	894	LYS
1	A	896	THR
1	A	901	SER
1	A	902	GLU
1	A	943	THR
1	A	945	LEU
1	A	952	LEU
1	A	955	GLU
1	A	959	LEU
1	A	960	ASP
1	A	972	LEU
1	A	975	ARG
1	A	982	LEU
1	A	986	VAL
1	A	988	LEU
1	A	994	VAL
1	A	998	LYS
1	A	999	GLN
1	A	1001	GLU

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Mol	Chain	Res	Type
1	A	1006	LYS
1	A	1021	THR
1	A	1034	ARG
1	A	1038	THR
1	A	1040	LYS
1	A	1046	ILE
1	A	1047	CYS
1	A	1051	LEU
1	A	1056	ILE
1	A	1062	LEU
1	A	1074	LEU
2	B	4	ILE
2	B	20	CYS
2	B	27	LYS
2	B	32	GLU
2	B	33	VAL
2	B	35	VAL
2	B	55	LEU
2	B	73	SER
2	B	77	THR
2	B	83	CYS
2	B	113	ILE
2	B	121	LEU
2	B	127	THR
2	B	131	LEU
2	B	133	LYS
2	B	134	MET
2	B	162	LYS
1	E	715	ASN
1	E	717	GLN
1	E	722	LYS
1	E	724	VAL
1	E	731	ARG
1	E	750	LEU
1	E	758	LEU
1	E	766	LYS
1	E	778	LEU
1	E	797	LYS
1	E	798	LYS
1	E	799	LEU
1	E	807	LYS
1	E	809	ILE

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Mol	Chain	Res	Type
1	E	822	ARG
1	E	831	GLN
1	E	838	ILE
1	E	843	ILE
1	E	855	LEU
1	E	871	LEU
1	E	873	ASP
1	E	876	ILE
1	E	879	MET
1	E	882	LEU
1	E	884	LYS
1	E	887	LEU
1	E	888	LEU
1	E	890	GLU
1	E	918	LYS
1	E	926	GLN
1	E	940	LEU
1	E	945	LEU
1	E	964	ARG
1	E	965	LYS
1	E	967	ILE
1	E	973	THR
1	E	975	ARG
1	E	978	LYS
1	E	981	THR
1	E	986	VAL
1	E	988	LEU
1	E	997	GLN
1	E	998	LYS
1	E	1004	LEU
1	E	1010	LYS
1	E	1036	VAL
1	E	1055	GLN
1	E	1056	ILE
1	E	1059	LEU
1	E	1065	SER
1	E	1068	ASN
1	E	1074	LEU
1	E	1079	ARG
2	F	4	ILE
2	F	7	LYS
2	F	8	LEU

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Mol	Chain	Res	Type
2	F	11	VAL
2	F	21	LEU
2	F	28	ASP
2	F	32	GLU
2	F	35	VAL
2	F	51	LYS
2	F	55	LEU
2	F	80	ILE
2	F	86	ILE
2	F	90	ASP
2	F	100	THR
2	F	113	ILE
2	F	131	LEU
2	F	134	MET
2	F	162	LYS
2	F	168	ARG
2	F	180	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	715	ASN
1	A	718	HIS
1	A	863	HIS
1	A	880	GLN
2	B	41	ASN
1	E	717	GLN
1	E	865	GLN
1	E	903	HIS
1	E	931	HIS
1	E	950	ASN
1	E	997	GLN
2	F	52	GLN
2	F	126	HIS

5.3.3 RNA ⓘ

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

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	355/418 (84%)	0.09	14 (3%) 43 34	38, 65, 108, 130	0
1	E	358/418 (85%)	0.13	15 (4%) 40 32	38, 66, 110, 133	0
2	B	178/178 (100%)	-0.11	3 (1%) 69 62	40, 58, 98, 114	0
2	F	178/178 (100%)	-0.08	3 (1%) 69 62	40, 61, 98, 112	0
All	All	1069/1192 (89%)	0.04	35 (3%) 49 39	38, 63, 106, 133	0

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	1053	PRO	4.7
1	E	1037	ALA	4.5
1	A	1037	ALA	4.2
1	A	1054	PRO	4.0
1	E	720	VAL	3.8
1	E	1038	THR	3.7
1	E	1051	LEU	3.6
1	A	1051	LEU	3.5
1	A	1053	PRO	3.5
1	A	1048	THR	3.5
1	E	1054	PRO	3.4
2	F	26	SER	3.2
1	A	1052	GLY	3.1
1	E	1081	ALA	3.0
1	E	1047	CYS	2.9
1	A	1038	THR	2.9
1	A	944	ALA	2.8
1	E	1048	THR	2.7
2	F	33	VAL	2.6
2	B	25	ASN	2.5
1	A	1021	THR	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	952	LEU	2.4
1	A	1081	ALA	2.4
2	F	30	PHE	2.3
1	A	720	VAL	2.3
1	E	952	LEU	2.2
1	E	1034	ARG	2.2
1	E	1055	GLN	2.1
1	E	981	THR	2.1
2	B	26	SER	2.1
1	A	1036	VAL	2.1
2	B	33	VAL	2.1
1	A	1047	CYS	2.0
1	E	1010	LYS	2.0
1	E	865	GLN	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.